

Geometric origin of mechanical properties of granular materials

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Model granular assemblies, in which grains are assumed rigid and frictionless, at equilibrium under some prescribed external load, are shown to possess, under generic conditions, several remarkable mechanical properties, related to isostaticity and potential energy minimization. Isostaticity – the uniqueness of the contact forces, once the list of contacts is known– is established in a quite general context, and the important distinction between isostatic *problems* under given external loads and isostatic (*rigid*) *structures* is presented. Complete rigidity is only guaranteed, on stability grounds, in the case of spherical cohesionless grains. Otherwise, the network of contacts might deform elastically in response to small load increments, even though grains are perfectly rigid. In general, one gets an upper bound on the contact coordination number. The approximation of small displacements, that is introduced and discussed, allows to draw analogies with other model systems studied in statistical mechanics, such as minimum paths on a lattice. It also entails the uniqueness of the equilibrium state (the list of contacts itself is geometrically determined) for cohesionless grains, and thus the absence of plastic dissipation in rearrangements of the network of contacts. Plasticity and hysteresis are related to the lack of such uniqueness, which can be traced back, apart from intergranular friction, to non-reversible rearrangements of small but finite extent, in which the system jumps between two distinct potential energy minima in configuration space, or to bounded tensile forces, deriving from a non-convex potential, in the contacts. Properties of response functions to load increments are discussed. On the basis of past numerical studies, it is argued that, provided the approximation of small displacements is valid, displacements due to the rearrangements of the rigid grains in response to small load increments, once averaged on the macroscopic scale, are solutions to elliptic boundary value problems (similar to the Stokes problem for viscous incompressible flow).

PACS numbers: 46.10.+z, 05.40.+j, 83.70.Fn

I. INTRODUCTION

A. Motivations

A large research effort, both in the statistical physics and the mechanics and civil engineering communities, is currently being devoted to granular materials, aiming in particular at a better understanding of the relationships between grain-level micromechanics (intergranular contact laws) and macroscopic behaviours (global equilibrium conditions, constitutive relations) [1, 2, 3].

This aim –the traditional program of Statistical Mechanics – is far from fully achieved in dense granular systems near equilibrium, for one is facing at least two fundamental difficulties.

Firstly, the non-smooth character of contact laws, that involve unilaterality and, possibly, dry friction, is a common feature of granular assemblies that endows them with a high level of disorder and a high sensitivity to perturbations. Tiny motions might significantly affect the way forces are transmitted, since contacts between neighbouring grains might open or close (and the sliding or non-sliding status of closed ones might change). Hence the characteristically heterogeneous aspect of force transport in dense granulates: large forces are carried by a network of preferred paths (the “force chains”) while

some grains or sets of grains carry but vanishing efforts (“arching effect”). The histogram of contact forces spans a wide range. These phenomena have been experimentally observed thanks to techniques like photoelastic stress visualization [4, 5] and carbon paper print analysis [6, 7]. They have also been studied in numerical simulations [8, 9], and some attempts of theoretical descriptions have been proposed [10]. Such peculiar aspects of granular systems render more difficult the reference to existing models from other fields. Indeed, a recent trend in the physics literature on static granular systems [11, 12, 13, 14] insists on their difference with ordinary, elastic solids, and suggests, instead of resorting to macroscopic displacement or strain variables, to search for direct relations between the components of the stress tensor.

The second basic difficulty stems from the incomplete knowledge of the mechanical properties of granular systems, especially those ruling the dynamics. When a granular sample is submitted to some prescribed external actions that are sufficiently slowly changing in time, its evolution is customarily described as an ordered set of equilibrium states that are successively reached, with little or no dependence on physical time. The physical processes by which kinetic energy is dissipated are, however, most often somewhat mysterious or poorly characterised. They are, in the framework of the *quasi-static* description we have just mentioned, implicitly regarded as irrelevant. One might wish to assess the validity of such an assumption. Numerical simulations, that have to adopt some rule to move the grains, could in principle allow useful

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investigations of the influence of the dynamics. However, in view of the practical difficulty to obtain representative configurations close enough to equilibrium within a reasonable computation time, they sometimes resort to non-physical parameters, and pick up the dynamical rule among the restricted range of those that allow tractable calculations.

This paper addresses both those basic concerns, in the following way. Simplifying assumptions are introduced (we consider, *e.g.*, rigid frictionless grains), thus restricting our attention to a certain class of model systems, that are however argued to exhibit the same qualitative behaviours as more realistic ones. Those systems are suitable candidates to test, most easily by numerical means, some recently proposed models and speculations, at the expense of rather extensive numerical computations. The purpose of the present article is not, however, to present new results of numerical simulations. We shall state and establish, rather, with a fair level of generality, some basic properties of such systems, and study their qualitative consequences in terms of macroscopic mechanical behaviour. This analysis will shed some light on some analogies and differences with other previously studied problems in statistical mechanics, such as directed ‘polymers’ in random environments and percolation models. It will also, along with the exploitation of past numerical results on a simplified model [9, 15, 16, 17, 18], allow us to investigate the possible origins of some macroscopic features of granular mechanics, that are classically modelled with elastoplastic constitutive laws [3, 19], and to discuss other recently proposed approaches [11, 12, 13, 14].

We will show that mechanics is to a large extent determined by geometrical aspects (steric exclusion), thus partially answering concerns about the role of dynamical parameters. Finally we will discuss the status of displacement and strain variables in quasi-static assemblies of rigid grains, and give perspectives for future investigations.

B. Synopsis.

The paper is composed of two main parts.

First, sections II to V introduce useful definitions and state basic properties that are necessary for the derivation of the main results.

Thus, section II presents useful definitions and mechanical properties of static granular systems, *i.e.*, collections of rigid bodies essentially interacting via point forces mutually exerted on their surfaces. Those notions, that include the theorem of virtual power, generalized forces and velocities for collective degrees of freedom, and the degree of indeterminacy of forces and of velocities, are not always familiar in the condensed matter physics community. Section III introduces the potential energy minimization problems for various simple frictionless contact laws. Section IV defines the approximation of small displacements, a modelling step of both technical

and conceptual importance, since it allows, in particular, an analogy with problems of scalar transport on discrete networks, as explained in section V.

Once those essential ingredients made available, the second part of the paper (sections VI to IX) establishes the main results and discusses their consequences, with reference to previous theoretical and numerical work, and to known aspects of the mechanical behaviour of granular materials.

Section VI is devoted to the *generic isostaticity property* of equilibrium states in systems of rigid grains that may only exert normal contact forces on one another. We then prove and discuss (section VII) the *uniqueness* of the equilibrium state in cohesionless systems within the approximation of small displacements, and compare the determinatin of equilibrium states of such systems with other mechanical or scalar transport problems. Section VIII introduces the additional requirement of stability, outside the approximation, which is dealt with, in the absence of friction, in terms of potential energy minimization. In some restricted models, this allows to conclude to the isostaticity of the structure, a stronger property than mere isostaicity of the problem under a given load. It is then possible to discuss the possible origins of plasticity in systems of frictionless grains and the form of the mechanical response to small load increments. The paper ends with concluding remarks (X) on the role of displacements and strains in granular materials and suggestions for future research.

II. BASIC DEFINITIONS AND PROPERTIES.

We are interested in the modelling of large packings of solid bodies (grains), in equilibrium under some prescribed external forces. Grains are assumed to interact *via* point forces mutually exerted on their surfaces, which means that the distribution of stress on their areas of contact or of influence can effectively be viewed as localized at a point, on the scale of the whole grain. Apart from this reservation, that excludes flat or conforming surfaces [56], grains might have arbitrary shapes, and our considerations apply to spatial dimension d equal to 2 or 3, although most examples will be taken with two-dimensional systems of discs. Note that we do not require interacting grains to touch one another at this stage. We mostly restrict our attention here to *frictionless* bodies, *i.e.*, such that contact forces are normal to the grain surfaces. This might look like a severe limitation, but we shall argue that such simplified systems do possess the generic properties of granular media. We shall also assume, unless otherwise specified, that the grains behave as rigid undeformable objects.

A. System, external forces

We consider a set of n grains, labelled with indices i , with $1 \leq i \leq n$. In each of them we arbitrarily choose a ‘center’, which might *e.g.*, coincide with its center of mass. In the case of spherical grains it is of course convenient to take the geometrical center of the sphere. The (d -dimensional) velocities of those centers, $(\mathbf{V}_i)_{1 \leq i \leq n}$, together with the d' -dimensional (with $d' = \frac{d(d-1)}{2}$) angular velocities $(\boldsymbol{\Omega}_i)_{1 \leq i \leq n}$, make up the kinematic degrees of freedom of the whole system, thus labelled by couples of indices (i, α) , with $1 \leq i \leq n$ and $1 \leq \alpha \leq d+d' = \frac{d(d+1)}{2}$. We denote as I the set of such couples. If $\alpha > d$, $V_{i,\alpha}$ is now a notation for $\Omega_{i,\alpha-d}$. Boundary conditions are often enforced by prescribing the motion, or the absence of motion, of walls. Those might be regarded as solid bodies, or particular ‘grains’ themselves. In the following we shall sometimes write down large ‘velocity vectors’ that gather all N_f kinematic degrees of freedom of the system, then denoted, with a single index, as $(v_\mu)_{1 \leq \mu \leq N_f}$.

It might also be convenient to keep some grain coordinates fixed (thus choosing one particular Galilean frame), *i.e.*, to impose, for all couples i, α belonging to some subset I_0 of I , $V_{i,\alpha} = 0$. Indices μ are then renumbered, and N_f is reduced accordingly, to label and to count the free kinematic parameters. Another classical way to impose some boundary conditions is to require, for all i, α in some subset I_1 of I , $V_{i,\alpha}$ to depend linearly on one or several parameters, *e.g.*:

$$(i, \alpha) \in I_1 \quad V_{i,\alpha} = A_{i,\alpha} \lambda_1, \quad (1)$$

introducing some collective ‘generalized velocity’ λ_1 . Once again, in such a case, N_f is reduced to count elements of $I \setminus (I_0 \cup I_1)$, plus λ_1 .

At least locally, it is possible to regard velocities and generalized kinematic parameters (like λ_1 in eqn. 1) as time derivatives of spatial coordinates, which we shall do in the following, thus writing, *e.g.*, $V_{i,\alpha} = \frac{dX_{i,\alpha}}{dt}$. As we are only interested in those properties that do not depend on dynamics, grain trajectories might as well be described by any parameter, not necessarily by physical time. In the case of kinematic constraints of type 1, parameters $A_{i,\alpha}$ will be regarded as fixed, although positions of the grains and the walls change. One then defines a generalized coordinate Λ_1 , such that $\frac{d\Lambda_1}{dt} = \lambda_1$. Just like for velocities, the compact notation $(x_\mu)_{1 \leq \mu \leq N_f}$ refers to the whole set of positional coordinates.

External forces and torques may at will be exerted on the grains that are free of kinematic constraints. We shall use the same notations as for velocities, writing down large N_f -vectors of ‘external forces’ (some of their coordinates standing, actually, for torques), as $(F_\mu^{ext})_{1 \leq \mu \leq N_f}$. At equilibrium, they are of course to be balanced by internal forces $(F_\mu^{int})_{1 \leq \mu \leq N_f}$:

$$(1 \leq \mu \leq N_f) \quad F_\mu^{ext} + F_\mu^{int} = 0. \quad (2)$$

In order to enforce constraints of type 1, some external efforts have to be exerted on the concerned bodies. On requiring the power of such efforts to be balanced by that of internal forces $(F_\mu^{int})_{1 \leq \mu \leq N_f}$, one identifies the generalized force conjugate to λ_1 as

$$Q_1 = - \sum_{(i,\alpha) \in I_1} F_{(i,\alpha)}^{int} A_{(i,\alpha)}. \quad (3)$$

We just used the power to find generalized forces: this is a manifestation of the *duality* between forces and displacements or velocities, which will be repeatedly exploited in the sequel. The N_f -dimensional vector space \mathcal{F} of external forces, is, by construction, to be regarded as the dual space, in the ordinary sense of linear algebra, of the N_f -dimensional space \mathcal{V} of kinematic degrees of freedom.

In general, it should be appreciated that the appropriate mathematical description of configuration space is not \mathbb{R}^{N_f} with its Euclidean structure, but, due to rotational degrees of freedom, an N_f -dimensional manifold, on which $(x_\mu)_{1 \leq \mu \leq N_f}$ is a set of (local) curvilinear coordinates. \mathcal{V} and \mathcal{F} are respectively the tangent and cotangent vector space at a given point, and depend on that point. Thus the definition of ‘constant velocities’, or of ‘constant forces’ requires some care. However, these difficulties are inessential in our subsequent treatment, and we shall assume ‘constant external forces’ are applied, and derive from a potential energy:

$$W = - \sum_{\mu=1}^{N_f} F_\mu^{ext} x_\mu. \quad (4)$$

It is easily checked that such a definition is devoid of ambiguity in the following important cases.

- The set of grain center positions, as opposed to grain orientations, define a ‘flat’ space, on which constant vectors and covectors are unambiguous. Whenever external efforts are not sensible to orientational coordinates, as in the case of gravity (if the grain ‘centers’ are their centers of mass), one may therefore ‘apply constant forces’.
- Anticipating on part IV, the approximation of small displacements assumes that the manifold might locally be replaced by its flat tangent space.

The complete N_f -vector of external forces is referred to as the *load*. Sometimes, it is convenient to deal with parametrized sets of loads. When the direction of the load is fixed, while its intensity might vary, one has a *one-parameter loading mode*. In such a situation, all external force components are kept proportional to a single loading parameter Q , and a generalized velocity conjugate to Q , λ , can be identified on equating the power of external forces with the product $Q\lambda$. λ is some linear combination of the kinematic degrees of freedom $(v_\mu)_{1 \leq \mu \leq N_f}$, and the time derivative of a generalized coordinate Λ , equal to

the same combination of coordinates $(x_\mu)_{1 \leq \mu \leq N_f}$. The potential energy is then simply

$$W = -Q\Lambda. \quad (5)$$

Let us now illustrate those notions with simple examples, that will be repeatedly used in the following. Systems A and B are packings of discs that are placed on the sites of a regular triangular lattice. (Later on, we shall allow for a slight polydispersity of the grains. They might move, gain or lose contacts with their neighbours, and the lattice might be slightly distorted). System A (fig.1) is a pile with slope inclined at 60 degrees with respect to the horizontal direction. Each disc is submitted

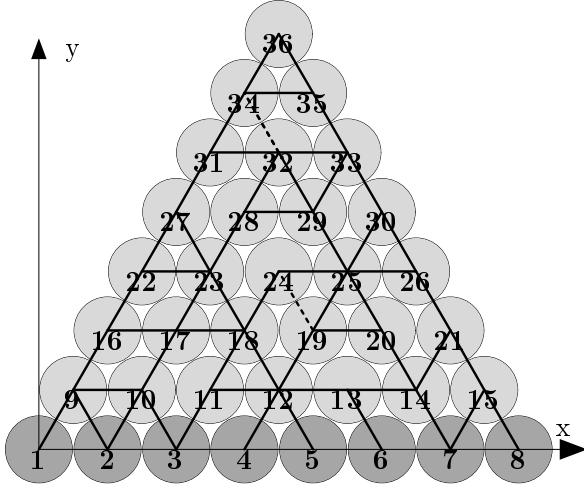


FIG. 1: System A : a pile under gravity. The bottom boundary conditions are explained in the text

to its own weight, except those of the bottom row, which collectively set the boundary condition. One might keep them fixed at regularly spaced positions, imposing, say (numbering them as on the figure, and denoting as a the lattice spacing)

$$(1 \leq i \leq 8) \begin{cases} x_i = (i-1)(1-\Lambda_1)a \\ y_i = 0 \end{cases}, \quad (6)$$

allowing for a horizontal deformation parameter Λ_1 . One may also require them to stay on the horizontal axis $y = 0$ and satisfy

$$v_i^y = -\lambda_1(i-1)a, \quad (7)$$

with a free kinematic parameter λ_1 . According to eqn. 3, the generalized force conjugate to λ_1 is

$$Q_1 = \sum_{i=1}^8 F_{i,x}^{int}(i-1)a. \quad (8)$$

These two slightly different boundary conditions (BC) are respectively abbreviated as BC1 and BC2 in the following.

System B (fig. 2) is a hexagonal sample of the same material. It is submitted to external forces on the periphery, which mimic hydrostatic pressure.

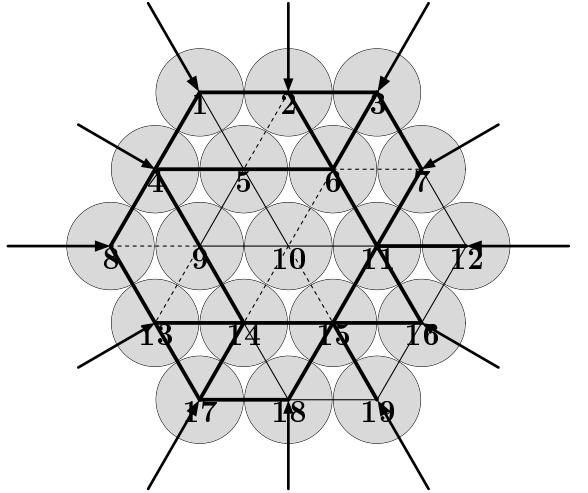


FIG. 2: System B : a hexagonal sample. Arrows depict external forces applied on peripheral discs.

System C (fig. 3) is a disordered collection of discs with a larger polydispersity. It is embedded within a circular wall the radius R of which might change. One controls the generalized force conjugate to $\lambda_1 = \frac{dR}{dt}$, *viz.*

$$Q_1 = \sum_i f_{iw}, \quad (9)$$

where the sum runs over all particles i exerting forces f_{iw} normally onto the wall.

B. The structure: a set of bonds.

The definitions we introduce here pertain to one specific configuration of the grains, with the positions and orientations fixed.

We call ‘bonds’ the pairs of neighbouring grains that *may* exert a force on one another. We require this force to be concentrated at the point of each grain which is the closest to the other one, and directed normally to the surface.[57] The more general case of arbitrary bond forces will be briefly evoked later. Note that we neither require the grains that are joined by a bond to be in contact, nor impose any sign constraint on the force. We thus define, somewhat arbitrarily at this stage, N such bonds as depicted on figure 4, alternatively labelled with an index l , $1 \leq l \leq N$, or with the pair of labels of the two grains they join. If bond l connects i and j , \mathbf{n}_l or \mathbf{n}_{ij} denotes the unit vector that points from i to j , normally

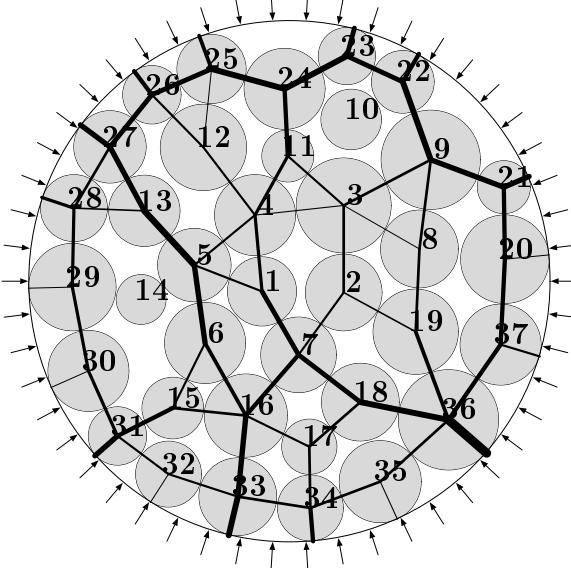


FIG. 3: System C : a disordered packing surrounded by a circular wall that might uniformly expand or shrink, as indicated by the small arrows.

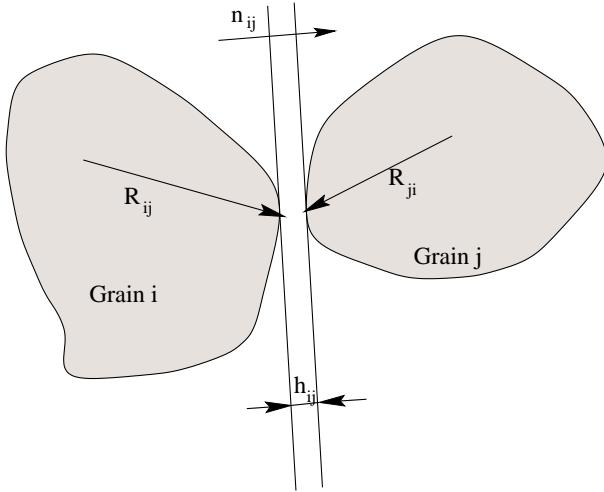


FIG. 4: Two grains i and j joined by a bond. h_{ij} is the minimum distance between their surfaces, measured where a common normal unit vector is \mathbf{n}_{ij} . Vector \mathbf{R}_{ij} (respectively \mathbf{R}_{ji}) points from the center of i (resp. of j) to the point of its surface that is closest to j (resp. to i)

to the surfaces of both grains where the distance between them, h_{ij} , is the smallest. \mathbf{R}_{ij} is the vector joining the center of grain i (origin), to the point on its surface that is closest to grain j (extremity). This contact zone might transmit a *normal* force, along \mathbf{n}_{ij} , of magnitude f_{ij} that will be counted positively when the grains repel each other. Once this set of bonds is defined, it is referred to as the *structure*. The set of bonds defined by intergranular contacts ($h_{ij} = 0$) will be called the *contact structure*.

As a consequence of the definition of a structure,

the form of internal forces ($(\mathbf{F}_i^{int})_{1 \leq i \leq n}$) and torques ($(\mathbf{\Gamma}_i^{int})_{1 \leq i \leq n}$) in the system is specified: they linearly depend on bond forces f_{ij} , as

$$\begin{aligned}\mathbf{F}_i^{int} &= - \sum_{j \neq i} f_{ij} \mathbf{n}_{ij} \\ \mathbf{\Gamma}_i^{int} &= - \sum_{j \neq i} f_{ij} \mathbf{R}_{ij} \wedge \mathbf{n}_{ij}.\end{aligned}\quad (10)$$

Given the load $(F_\mu^{ext})_{1 \leq \mu \leq N_f}$, equilibrium requires, in view of eqns. 10 and 2 that the bond forces $(f_l)_{1 \leq l \leq N}$ satisfy equations of the form

$$(1 \leq \mu \leq N_f) \quad \sum_{l=1}^N H_{\mu l} f_l = F_\mu^{ext}, \quad (11)$$

defining a linear operator, $H : \mathbb{R}^N \rightarrow \mathcal{F}$. Bond forces $(f_l)_{1 \leq l \leq N}$ are then said to be *statically admissible* with the load $(F_\mu^{ext})_{1 \leq \mu \leq N_f}$. Bond forces that are statically admissible with a load equal to zero (in equilibrium without any external action) are the elements of a subspace S_0 of \mathbb{R}^N , the null space of operator H . Its dimension, that we denote as h , is the number of linearly independent such self-balanced sets of internal forces, or, in other words, the *degree of indeterminacy of bond forces* in the system (also called the *degree of hyperstaticity*). If not empty, the set of statically admissible bond forces is an affine space of dimension h .

The relative normal velocity of the grains i and j joined by a bond is

$$\delta V_{ij} = \mathbf{n}_{ij} \cdot (\mathbf{V}_i - \mathbf{V}_j + \boldsymbol{\Omega}_i \wedge \mathbf{R}_{ij} - \boldsymbol{\Omega}_j \wedge \mathbf{R}_{ji}), \quad (12)$$

with the convention that it is positive when the particles are approaching each other. Eqn. 12 defines a linear operator, G , acting on \mathcal{V} into \mathbb{R}^N . The *range* of G is the subspace \mathcal{C} of *compatible* relative normal velocities, *i.e.*, those N -vectors for which one can effectively find values for the velocities, relations 12 being satisfied. The *null space* of G is the vector space M of ‘mechanisms’, also called ‘floppy modes’, *i.e.*, motions that do not alter the lengths h_l of the bonds. Its dimension, denoted as k in the sequel, is the number of independent such motions, or, in other words, regarding the bonds as rigid, the *degree of indeterminacy of velocities*, also called *degree of hypostaticity*. Imposing the condition $\delta V_{ij} = 0$ in all bonds of the structure restricts the possible values of velocities $(v_\mu)_{1 \leq \mu \leq N_f}$ to a vector space of dimension k . Depending on the type of load and boundary conditions, the whole set of grains might keep some overall rigid body kinematic degrees of freedom. System B, for instance, has 3 independent such motions, as any solid body in 2D. If $k_0 \leq d(d+1)/2$ denotes the number of such particular motions allowed by the boundary conditions, the system is said to be *rigid* when it does not have other mechanisms, *i.e.*, when $k = k_0$.

An important and useful result, the classical *theorem of virtual power* states the following. Let $(\delta V_l)_{1 \leq l \leq N}$ be

any element of \mathcal{C} , corresponding to the velocity vector $(v_\mu)_{1 \leq \mu \leq N_f}$, and let $(f_l)_{1 \leq l \leq N}$ be a set of bond forces statically admissible with the load $(F_\mu^{ext})_{1 \leq \mu \leq N}$. One then has:

$$\sum_{l=1}^N f_l \delta V_l = \sum_{\mu=1}^{N_f} F_\mu^{ext} v_\mu. \quad (13)$$

Equality 13, for arbitrary ('virtual') equilibrium set of internal forces and velocities, stresses the *geometric* meaning of forces and the *mechanical* meaning of velocities. It is easily established in two steps: first use the force balance equations in the right-hand side; then transform the sum over degrees of freedom into a sum over bonds.

As a direct consequence of the theorem, one deduces that operator H is in fact (as one might check directly, reading the matrix elements in eqns. 12 and 11) the transpose of G : $H = G^T$. This follows from the sequence of equalities

$$(f|\delta V) = (f|Gv) = (Hf|v) = (G^T f|v),$$

valid for arbitrary v (such that $Gv = \delta v$) and f (such that $Hf = F^{ext}$), in which a bracket notation is used for scalar products. Consequently, S_0 , the null space of G^T , is the orthogonal complementary to \mathcal{C} , the range of G , in \mathbb{R}^N :

$$S_0 = \mathcal{C}^\perp. \quad (14)$$

Thus to check that some values δV_l that one might try to assign to the relative normal velocities are compatible, it is sufficient to ensure the orthogonality of N -vector $(\delta V_l)_{1 \leq l \leq N}$ to all N -vectors of self-balanced bond forces (or a spanning subset thereof):

$$(\delta V_l)_{1 \leq l \leq N} \perp S_0. \quad (15)$$

One thus uses *forces* (elements of S_0) as cofactors in a set of *geometric* compatibility conditions.

Recalling k (the number of mechanisms) is the dimension of the null space M of G , one has

$$N_f = k + \dim(\mathcal{C}).$$

As $h = \dim(S_0)$, from 14, one also has:

$$N = h + \dim(\mathcal{C}).$$

Elimination of the dimension of \mathcal{C} from those two equalities yields the following relationship between the degree of hypostaticity, k , the degree of hyperstaticity, h , the number of bonds, N , and the number of degrees of freedom, N_f :

$$N + k = N_f + h. \quad (16)$$

As we will check on examples below, relation 16 holds whatever the choice of the list of bonds between objects, although it is of course desirable in practice to define

bonds according to the interaction law. One may, for example, declare a bond to join two grains whenever their surfaces are separated by a minimum distance smaller than some threshold $h_0 > 0$. The choice of a larger h_0 , thereby increasing N , will decrease k and/or increase the degree of hyperstaticity h .

Let us remark that the properties we have just dealt with in the case of bonds that carry normal forces, are very easily generalized to the case of arbitrary contact forces, at the cost of minor modifications. Relative normal velocities and normal contact forces are replaced by d-vectors, \mathbb{R}^{dN} replaces \mathbb{R}^N , equalities 13 (with, now, a scalar product within the sum in the left-hand side) and 14 are still satisfied. Instead of 16, one ends up with $dN + k = N_f + h$. Adding friction increases h and/or decreases k .

Returning to frictionless systems, the case of spheres or discs deserves a special treatment: no normal force is able to exert any torque, and all rotational degrees of freedom are therefore mechanisms. It is convenient to ignore them altogether. Their number $n \frac{d(d-1)}{2}$ (n is the number of particles) is then subtracted both from N_f and from k , and eqn.16 still holds. Such granular systems are then analogous to 'central-force networks': networks of freely articulated bars, or systems of threads tied together, in which only the translational degrees of freedom of the nodes matter. One should be aware, however, that the presence of friction reinstates rotations into the problem.

We now illustrate the notions and properties introduced in this section with examples of structures defined in systems A, B and C, ignoring, as explained just above, disc rotations.

First consider system B. Three different structures are apparent on figure 2. The first one, that we denote as SB1, is the set of bonds that are drawn as thick lines; the second, SB2, contains all bonds of SB1, plus those that are drawn with thin continuous lines on the figure; and, finally, the third structure, SB3, comprises all possible bonds between nearest neighbours in the system, i.e., all those of SB2 plus the dotted lines. Ignoring rotations, one has $N_f = 2n = 38$.

Structure SB3 is a set of rigid triangles sharing common edges with their neighbours. It is devoid of mechanisms, except the 3 overall rigid body degrees of freedom of the system. Thus $k = 3$. $N = 42$ bonds are present. In view of eqn. 16, one has $h = 7$. One can exhibit 7 linearly independent systems of self-balanced normal forces, as follows. The small structure, with 12 bonds, involving 7 discs, depicted on fig. 5, allows to define one such set of forces. Noting that 7 such patterns are present on SB3 (centered on discs 5, 6, 9, 10, 11, 14 and 15), the right count is reached.

Structure SB2 is made of $N = 35$ bonds. It can be shown (on studying the properties of the corresponding matrix G) to be devoid of self-balanced sets of forces, $h = 0$, and of mechanisms other than rigid body motions, $k = 3$. Thus $N + k = N_f + h$.

Structure SB1, comprising $N = 25$ bonds only, still

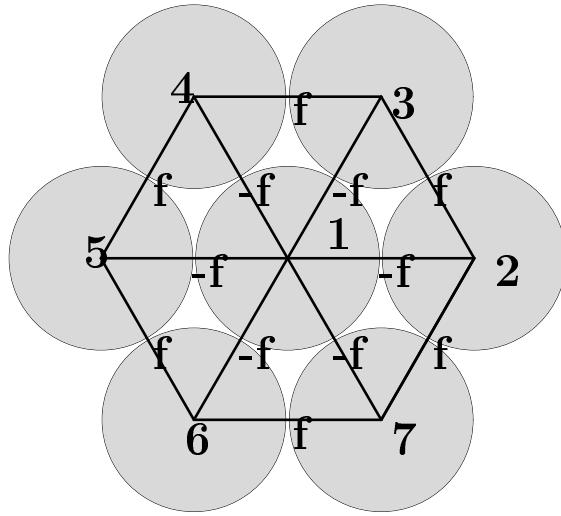


FIG. 5: A set of self-balanced normal forces. The 6 bonds of the regular hexagon perimeter carry some normal force f , while the 6 ones involving the central disc labelled 1 carry the opposite force.

has $h = 0$. According to eqn. 16, it should possess 10 additional independent mechanisms. 2 of them are due to disc 10, which is now completely free. 4 others involve discs 5, 9, 12, and 19, which are still free to move in one direction. In the case of a divalent disc like 5, this is due to the exact alignment, on the regular lattice, of bonds 4-5 and 5-6. Four less trivial mechanisms are more collective. One of them is shown on figure 6. Two structures,

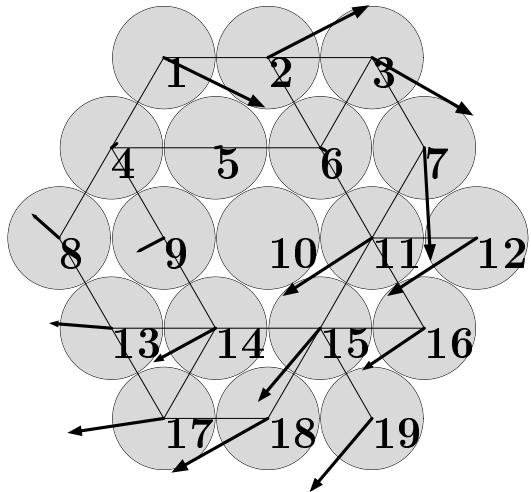


FIG. 6: A collective mechanism on structure SB1. Arrows represent disc velocities.

SA1 and SA2, are defined, on fig. 1, in system A. SA1 is made of all bonds drawn with continuous lines, and SA2

contains, in addition, the two bonds drawn with dotted lines (19-24 and 32-34). Depending on the boundary condition, discs 1 to 8 either possess collectively one degree of freedom (for BC2) and then $N_f = 57$, or none (for BC1) and $N_f = 56$.

SA2 has 57 bonds. It is devoid of mechanism ($k = 0$) for whatever BC. For BC2, one also has $h = 0$ and eqn.16 holds as an equality between the number of bonds and the number of degrees of freedom. For BC1, one has $h = 1$. Indeed, one may recognize, in the bottom left corner of the pile, with discs 1, 2, 3, 9 and 10, part of the hyperstatic pattern of fig. 5. With BC1, one needs not care about equilibrium of discs 1, 2 and 3 that are perfectly fixed. A system of self-balanced bond forces is thus found on attributing a common value to the normal forces in bonds 1-9, 9-10, 10-3, and the opposite value to the normal forces in bonds 2-9 and 2-10. In the case of BC2, those forces do not balance, since the equilibrium equation for the collective degree of freedom of the bottom row (a combination of eqns. 8 and 10) is not satisfied. As to SA1, it has the same properties as SA2, with 2 additional mechanisms (collective ones like that of fig. 6).

Consider now structure SC that is shown, in system C, on figure 3, with the lines connecting disc centers, or joining discs to the wall, that define $N = 70$ bonds. Taking into account the degree of freedom of the wall, one has $N_f = 2n + 1 = 75$. One may show $h = 0$. Thus one has $k = 5$. Two discs (10 and 14) are entirely free, hence 4 mechanisms. The missing one is a global rotation, as a solid body, of the set of all particles around the center of the circular container, the wall remaining immobile. Such a motion would not be possible if the same boundary condition was used with another container shape.

C. The problem: the structure and the load.

Once a list of bonds is chosen, thus defining the structure, we shall refer to the situation of the structure submitted to a given load as ‘the problem’.

Solving the problem would mean finding the motion or equilibrium state of the system (determining, *e.g.*, new equilibrium positions and intergranular forces), once the load, from an initial state of rest with no external force, has been applied. We are not, of course, able to do that at this stage, since no contact law relating the forces to the relative motion of neighbouring particles has been introduced. The only information available is that the internal forces are required to belong to some vector space that is known once the structure is defined, and to be exerted on given points on the grain surfaces.

It is said that *the load is supported* by the structure if its application leads to an equilibrium state in which internal forces, carried by the bonds of the structure, balance the external ones.

We can state a necessary condition for the load to be supported: it must be possible to find statically admissible

sible intergranular forces. Necessarily, the N_f -vector of external forces must lie in the range of operator G^T , i.e., it must be orthogonal to the null space M of G :

$$(F_\mu)_{(1 \leq \mu \leq N_f)} \perp M. \quad (17)$$

This simply means that if the load is to be supported, it must not set the mechanisms into motion. Such a load is said to be *supportable*. All supportable loads are not always supported.

By definition, the *backbone* of a structure is the set of bonds l_0 such that a list of statically admissible internal forces $(f_l)_{1 \leq l \leq N}$ exists with $f_{l_0} \neq 0$. In the following we shall also refer, as ‘the backbone’, to the set of grains reached by such bonds.

In general, a full mechanical characterization of the equilibrium properties of the system requires some constitutive law in the contacts. However, there are interesting situations in which

- condition 17 being fulfilled, the load is supportable;
- if it is supported, then all intergranular forces are uniquely determined by the equations of equilibrium.

These two conditions define an *isostatic problem*.

Further restrictions on internal forces are often enforced in the form of inequalities. The definition of a supportable load is then modified accordingly, imposing additional conditions, to be satisfied simultaneously with 17. Their consequences will be discussed in sections III and VII.

D. Isostaticity: various definitions.

In section VI we shall see that equilibrium configurations of assemblies of rigid frictionless grains interacting via contact forces only are generally such that the problem is isostatic.

Here, we first insist on the difference between an *isostatic problem*, as defined just above, and an *isostatic structure*, to be defined below. Once condition 17 is satisfied, the set of possible bond forces is an affine space of dimension h . One has an isostatic problem if both conditions 17 and $h = 0$ are fulfilled. Some mechanisms might still exist in the structure ($k \neq 0$), provided they are orthogonal to the load direction.

Structure SA1 (figure 1), with discs exactly centered on the sites of a regular triangular lattice, is such that the problem, denoted as PA1 in the following, defined with BC2 and the following load: [58]

$$\left\{ \begin{array}{l} (9 \leq i \leq 36) \quad \mathbf{F}_i^{ext} = -p\mathbf{e}_y \\ Q_1 = \frac{294}{5\sqrt{3}}p, \end{array} \right. \quad (18)$$

where p is the weight of one disc and \mathbf{e}_y is the vertical upwards unit vector, is isostatic, although 2 mechanisms are present.

Analogously, structure SB1, along with the load shown on figure 2, defines an isostatic problem PB1 in spite of the $k = 10$ mechanisms. In particular, the load direction (provided discs sit right on the regular lattice sites) is exactly orthogonal to the velocity vector represented on figure 6. Structure SC, submitted to the following load:

$$\left\{ \begin{array}{l} (1 \leq i \leq 37) \quad \mathbf{F}_i^{ext} = 0 \\ Q_1 = Q_1^0, \end{array} \right. \quad (19)$$

where a prescribed value Q_1^0 is imposed to generalized force Q_1 defined in eqn. 9, yields an isostatic problem.

Isostatic *structures*, on the other hand, are such that all problems are isostatic, whatever the choice of the load. More precisely, one requires all loads orthogonal to the overall rigid-body degrees of freedom to be supportable with a unique determination of internal forces. Equivalently, both conditions $h = 0$ and $k = k_0$ are to be satisfied. Both the degree of hyperstaticity and the degree of hypostaticity (excluding rigid-body motions) should be equal to zero. This entails the well-known condition

$$N = N_f - k_0, \quad (20)$$

stating that the number of equilibrium equations ($N_f - k_0$) is equal to the number of unknowns (N).

Equality 20 is a necessary condition for the structure to be isostatic, not a sufficient one. For example, in the structure defined by the addition of the bond joining discs 19 and 24 to SA1 with the first boundary condition (BC1), one has $k_0 = 0$, $N = N_f = 56$, while $h = k = 1$.

Structure SA2, with BC2, is isostatic. SB2, with $N_f = 38$ and $k_0 = 3$, is isostatic. As to SC, it would be isostatic upon removal of grains 10 and 14, only if the global rotation of the set of grains with respect to the wall were ignored. Of course, all those structures, as we are dealing with discs, are only isostatic if rotations are ignored. Only problems with no external torque exerted on the grains are isostatic. This should be remembered on comparing h and k with and without friction in such systems.

As we shall see, isostatic problems, rather than isostatic structures, naturally occur in some model granular systems. The distinction is relevant, for it accounts for disconnected or ‘dangling’ parts in disordered structures like SC, and for the peculiarities of lattice models. Moreover, some systems can also spontaneously, as we shall see, select a non-rigid ($k > k_0$) equilibrium configuration.

E. Generic versus geometric properties.

The distinction between isostatic problems and isostatic structures should not be confused with another one: that between *geometric* and *generic* isostaticity. We have used a *geometric* definition of a structure, as associated to one particular position of the system in configuration space, and accordingly the definition we gave

is that of geometric isostaticity. A *topological* one can be introduced which, irrespective of particle positions, is only sensitive to the connectivity of the network of bonds. In the case of spheres or discs, when rotations can be ignored, this amounts to regarding the structure as a graph: a set of edges (bonds) joining at vertices (grains). Operator G , spaces S_0 , M and their dimensions h and k smoothly depend on the coordinates of the grains, *via* vectors \mathbf{n}_{ij} and \mathbf{R}_{ij} . However, the rank of a parameter-dependent matrix stays at its maximum except for special values of the parameters. Equivalently, the dimension of the null space is generically equal to its minimum value. Applying this to both G and G^T , one may define the generic degree of indeterminacy of velocities (with due account to the k_0 rigid-body degrees of freedom) k and the generic degree of indeterminacy of forces h as the respective generic (minimum) dimensions of their null spaces. This allows to define a suitable isostaticity notion for topological structures: a *generically isostatic structure* is one for which both numbers h and $k - k_0$ are equal to zero.

It follows from the definitions that a geometrically isostatic structure is always, once regarded as a topological structure, a generically isostatic one, but that the reciprocal property is not true. Ref. [20] gives a counterexample for a system of discs (like systems A and B, equivalent to a network of articulated bars) on the regular triangular lattice. In specific configurations (like that of a regular triangular lattice), one might exceptionnally have $h = k - k_0 > 0$ on generically isostatic structures.

In two dimensions, there exists some powerful algorithms [21, 22] to evaluate the generic degrees of force and velocity indeterminacy in central-force networks (or systems of frictionless discs). Such computational methods only deal with connectivity properties, they do not manipulate floating-point numbers and are therefore devoid of numerical round-off errors. They were successfully applied to systems of up to 10^6 nodes. However they are of course unable to compute position-dependent quantities like force values.

III. CONTACT LAW AND POTENTIAL MINIMIZATION.

So far, the only restriction on intergranular forces was that they should be normal to the grain surfaces.[59] In this section we consider some more specific cases of frictionless grains, in which some “contact law”, relating normal forces to relative positions, is known. This provides some limited additional information, that is not sufficient in general to predict the grain trajectories once they are submitted to external forces, for all dynamical aspects are still unknown and the characterization of equilibrium might even be incomplete. Our aim is to deduce as much as possible on the global properties of the granular assembly from as little information as possible on the detailed mechanical laws of the contacts, in order to stress the

importance of geometrical aspects. Thus we first present the simplest case of rigid, frictionless and cohesionless grains, in which contacts simply behave as struts. Then we introduce and briefly discuss other possible laws in which unilaterality or rigidity constraints are modified or relaxed. Most of those frictionless systems possess a potential energy that is stationary at equilibrium states and reaches then a minimum if they are stable. Throughout this section, it is assumed that a one-parameter loading mode has been defined for varying particle positions and orientations, with constant external forces, and that the potential energy of external forces, W , can be written in the forms of eqns. 4 and 5.

A. Rigid frictionless grains, no cohesion.

In this case, the contact law takes the form of the so-called Signorini condition:

$$\begin{cases} f_{ij} = 0 & \text{if } h_{ij} > 0 \\ f_{ij} \geq 0 & \text{if } h_{ij} = 0 \end{cases} \quad (21)$$

It should be noted that this law does not express a functional dependence of f_l on h_l . Let us study the variations of W near equilibrium states. First, consider such a state, in which some non-negative contact forces f_l^* , in closed contacts ($h_l = 0$) balance the external load Q . Let us apply the theorem of virtual power with statically admissible force set $(f_l^*)_{1 \leq l \leq N}$, and arbitrary particle velocities, corresponding to relative normal velocities $\delta V_l = -\frac{dh_l}{dt}$ and a value $\lambda = \frac{d\Lambda}{dt}$ for the kinematic parameter conjugate to Q . For any l such that $f_l^* > 0$, the Signorini condition requires that $h_l = 0$ and one must have $\delta V_l \leq 0$ to comply with the impenetrability constraints. Then, from

$$\frac{dW}{dt} = -Q \frac{d\Lambda}{dt} = -Q\lambda = -\sum_l f_l^* \delta V_l$$

it follows that any motion that does not lead to grain interpenetration can only, to first order in t (any parameter on the trajectory in configuration space) *increase* the potential energy. This non-negative first-order variation might be equal to zero if $\delta V_l = 0$ for any active contact l , *i.e.*, if a mechanism exists on the backbone of the contact structure. Whether the equilibrium state corresponds to a minimum of W depends then on the sign of second or higher order variations. If the backbone of the contact structure is rigid, then W is necessarily minimized at equilibrium.

Conversely, let us assume that a configuration of the grains has been reached, that locally minimizes W under the constraints $h_l \geq 0$. There must then exist some non-negative *Lagrange multipliers* f_l , such that, for any coordinate x_α ,

$$-\frac{\partial}{\partial x_\alpha}(Q\Lambda) = -\sum_l f_l \frac{\partial h_l}{\partial x_\alpha}. \quad (22)$$

Only for such indices l that $h_l = 0$ do the f_l take non-vanishing values. The partial derivative in the right-hand side of 22 is the opposite of matrix element $G_{l,\alpha}$, while, from 4, that of the left-hand side is the external force conjugate to x_α . Thus, we have just written that parameters f_l are in fact equilibrium contact forces satisfying 21, and reaction forces stem from geometrical constraints.

We now introduce a few other related contact laws and mechanical models.

B. Systems with tensile or bilateral forces.

Networks of rigid strings or cables are analogous to frictionless spheres (ignoring their rotations) if the sign of forces is reversed and if the distance constraint $h_l \geq 0$ is replaced by $h_l \leq 0$. The Signorini condition 21 becomes

$$\begin{cases} f_{ij} = 0 & \text{if } h_{ij} < 0 \\ f_{ij} \leq 0 & \text{if } h_{ij} = 0, \end{cases} \quad (23)$$

and the whole treatment of the preceding subsection straightforwardly applies.

In the case of non-spherical grains, an analogous system supporting tensile forces is an idealized chain, in which ‘grain’-chain links- perimeters are free to cross. Pairs of neighbouring links (interpenetrating ‘grains’) exert a force on one another, opposing their separation, when their intersection reduces to a contact point.

A *bilateral* contact law:

$$\begin{cases} f_{ij} = 0 & \text{if } h_{ij} \neq 0 \\ f_{ij} \text{ unknown} & \text{if } h_{ij} = 0, \end{cases} \quad (24)$$

might model rigid cohesive grains, that ‘stick’ to one another. The sticking force might be limited by an inequality:

$$\begin{cases} f_{ij} = 0 & \text{if } h_{ij} \neq 0 \\ f_{ij} \geq -f_0 & \text{if } h_{ij} = 0, \end{cases} \quad (25)$$

When one simply uses the form 24, assuming the pairs that are stuck in contact will not come apart, the conclusions of subsection III.A still hold, if unilateral conditions on relative velocities and displacements are replaced by bilateral ones, and if all sign constraints on contact forces are removed. Equilibrium configurations are characterized by stationarity of potential energy W . Minimization of W ensures stability. A sufficient, but not necessary condition for minimization of W is the rigidity of the backbone of the contact structure.

Reciprocally, statically admissible normal contact forces naturally appear as Lagrange multipliers associated with bilateral constraints $h_l = 0$ at a potential energy minimum.

However, contact law 25 does not lend itself to a potential energy formulation.

Tensegrities[23] (with rigid elements) are by definition mixed networks of struts (satisfying condition 21) or bars

(bilateral) on the one hand, and cables (satisfying 23), on the other hand. Their potential energy has the same properties as stated above.

C. Systems with a smooth interaction potential.

The model of perfectly rigid grains is physically reasonable when contact deformations ($h_l < 0$) are negligible in comparison with any other relevant length in the problem. When this is no longer the case, or when one wishes to model sound propagation, it is appropriate to deal with contact laws that involve elastic deformations, e.g.,

$$\begin{cases} f_{ij} = 0 & \text{if } h_{ij} > 0 \\ f_{ij} = K_{ij}|h_{ij}|^m & \text{if } h_{ij} \leq 0, \end{cases} \quad (26)$$

in which K_{ij} is a stiffness constant that depends on material properties and on the geometry of contact i, j . The exponent is $m = 3/2$ (Hertz law) for smooth surfaces in 3D, and other values might model roughness and the presence of conical asperities [24, 25].

Such contact forces derive from an elastic potential energy:

$$W^{el} = \sum_{l=1}^N w(h_l), \text{ with } w(h_l) = \frac{K_l}{m+1} |h_l|^{m+1}. \quad (27)$$

Likewise, rigid cables as introduced in subsection III.B could be replaced by elastic ones. That stable equilibrium states correspond to minima, in the absence of frictions, of the total potential energy

$$W^{tot} = W^{el} + W, \quad (28)$$

sum of the elastic potential 27 and the potential energy of external forces 4 or 5, is an extremely familiar property. The Signorini condition might physically be regarded as the limit of the interaction law expressed by equation 26 when the stiffness constants become very large, or, equivalently, when the level of intergranular forces approaches zero. Alternatively, it is mathematically possible to introduce a regularized contact law of the form 26 as an approximation, when contacts are stiff enough, of the ideal impenetrability constraint. Such a point of view is adopted in optimization theory: the procedure known as penalization of the constraints amounts, instead of minimizing W subject to impenetrability constraints, to searching for unconstrained minima of $W + W^{el}$.

Tensile contact forces of limited intensity, as in contact law 25, might result from some attractive interaction of finite, but small, range, as depicted on fig. 7. It is interesting to note that the addition of an attractive tail has turned the potential $w(h)$ into a non-convex function of interstitial thickness h . At the inflexion point, A, the attractive force reaches its maximum f_A . If one pulls, with a growing force, on two grains in contact in order to

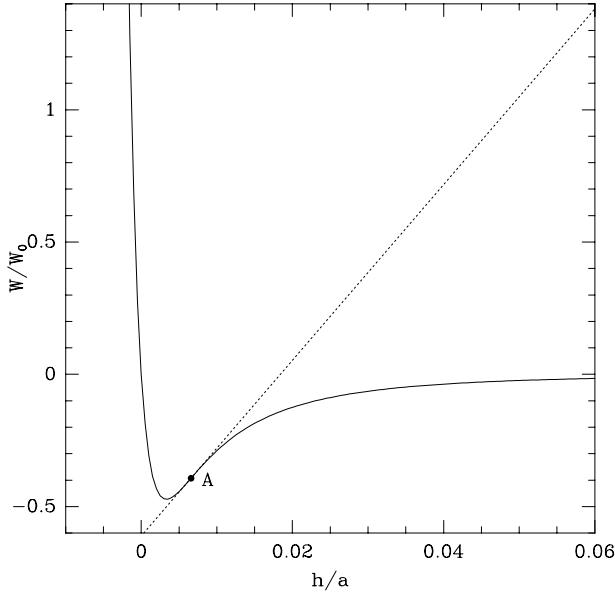


FIG. 7: Interaction potential, with an attractive tail, as a function of interstitial thickness h . The curve has an inflexion point A , corresponding to the maximum attraction force (equal to the slope of the dotted line).

separate them, an instability, in which the contact suddenly breaks open, is reached as the pulling force reaches the value f_A . When the corresponding intergranular distance, h_A , is so small that it is negligible in comparison to all other relevant lengths in the problem, one might then replace the smooth attractive potential by contact law 25, with $f_0 = f_A$. On doing so, one loses however the possibility to exploit minimization properties.

We shall see that the potential minimization properties have important consequences in terms of the possible uniqueness of the equilibrium state under a prescribed load, and, eventually, as to the possible origins of macroscopic plastic dissipation. But, first, we have to extend the properties we have stated for velocities (or infinitesimal displacements) to small displacements, around a given reference configuration.

IV. THE APPROXIMATION OF SMALL DISPLACEMENTS.

A. Definition.

We wish to use the concepts we have introduced in the preceding sections while allowing some motion of the grains, of small but finite extent, which might alter the list of closed intergranular contacts. Consequently, we introduce the assumption that displacements, from a reference configuration, are small enough as to be regarded as infinitesimal quantities. This *approximation of small displacements* (ASD) is a crucial step that is very often taken in solid state mechanics. Indeed, it is indispens-

able if one wishes to deal with linear problems: adding up two displacement fields, for instance, in continuum mechanics, is otherwise a meaningless operation. In the case of granular systems, it will also lead to a linearization of the problems, for the curvature of configuration spaces will be ignored. Its range of validity has to be assessed a-posteriori, but is of course presumably larger in dense systems, where contacts might open and close with only tiny changes of the relative positions of neighbouring grains.

Specifically, we assume the coordinates of the grains to stay close to reference values. Quantities pertaining to the reference configuration will be labelled with a superscript ‘0’. It is often convenient, then, to work with a fixed structure –the list of contacts that might close, and transmit a force, is a-priori known.

Interstitial thicknesses h_l are written as $h_l = h_l^0 - \delta u_l$, with a relative normal displacement δu_l that is *linear* in the grain displacements (and rotations), regarded as small quantities. Vectors \mathbf{n}_{ij} , \mathbf{R}_{ij} , \mathbf{R}_{ji} are regarded as constant, equal to \mathbf{n}_{ij}^0 , \mathbf{R}_{ij}^0 , \mathbf{R}_{ji}^0 . As they appear as cofactors of the displacements, taking their variations into account would introduce second order terms. All changes of the structure geometry are ignored. Spaces \mathcal{C} , \mathcal{S} , operators G , G^T , are assumed to be the same in the actual as in the reference configurations. Displacements are now endowed with the same linear algebraic structures as velocities. G operates on displacements, yielding relative normal displacements δu_l , the compatibility condition for relative normal displacements is the orthogonality to the space of self-balanced internal forces \mathcal{S}_0 , a theorem of virtual work can be stated instead of the theorem of virtual power, etc...

Within the framework of the ASD, the specificity of mechanical problems disappears: as the effect of the displacements of the grains (variations of the coordinates) on the positions (coordinates) themselves are ignored, one can find analogies with various other local properties of a list of fixed points, nodes or lattice sites. Forces now appear as unknown vectors carried by fixed directions, and the sum of incoming forces on a node has to vanish. Part V introduces the analogy with scalar transport on a fixed network.

B. Lattice models.

Regular packings of monodisperse spheres in 3D (or discs in 2D) on FCC or hexagonal compact (respectively, triangular in 2D) lattices are simple systems that are often studied theoretically, experimentally [26, 27] and numerically [9, 15, 16, 17, 28, 29, 30, 31, 32, 33]. Because truly monodisperse systems do not exist, and because of possible elastic deformations of the grains, one cannot expect such lattices to remain perfectly regular and undisturbed. However, as lattice perturbations will be small, it is a common practice [9, 15, 16, 17, 28, 29] to resort to the ASD, with a perfect lattice as the reference

configuration from which displacements and strains are evaluated.

Consider *e.g.*, the case of slightly polydisperse discs on a triangular lattice, as in systems A and B. A perfect lattice can be chosen as the reference state, in which the spacing between neighbouring sites is the lowest upper bound a of the diameter distribution. Diameters are assumed to be distributed between $a(1 - \alpha)$ and a , with a small parameter $\alpha \ll 1$. The diameter of disc i is thus

$$a_i = a(1 - \delta_i \alpha), \quad (29)$$

δ_i being a random number, drawn independently for each i between 0 and 1. When a certain number of intergranular contacts is created, as it is often necessary (cf. section III) in order to sustain some external forces, the lattice will be slightly distorted, with displacements of order α . The ASD amounts to deal with all relevant quantities to leading order in α . In all possible contacts, the normal unit vector is kept parallel to one of the three directions of dense lines in the triangular lattice. It is convenient to work with a fixed structure S_0 that comprises all bonds between nearest neighbours on the lattice. If grains are required to touch to exert a force on one another, forces, in a state of equilibrium under a supported load, will be carried by some contact structure, the bonds of which form a subset of S_0 .

One might then regard problem PA1, in system A, as defined on S_0 . Once the random radii were fixed, we found, within the ASD, an equilibrium configuration for problem PA1, satisfying the Signorini condition 21, in which the contact structure was SA1. Similarly, once the values of the radii were known in system B, SB1 was found, within the ASD, as the contact structure corresponding to a solution of problem PB1, posed on $SB3=S_0$. Within the ASD, all displacements and deformations are proportional to α , and the problem is, apart from a scale factor α for displacements, only sensitive to parameters $(\delta_i)_{1 \leq i \leq n}$.

Such is not the case, of course, without the ASD, if one takes into account the rotations of unit vectors \mathbf{n}_l of the bonds due to the deformation of the lattice.

V. ANALOGY WITH SCALAR PROBLEMS.

We briefly recall the analogy between the mechanical problems we have been discussing, within the approximation of small displacements, and that of current transport on a resistor network. Such an analogy was presented *e.g.*, in ref. [20]. It is useful because some properties are more immediately intuitive in scalar models, and because statistical models (percolation, directed percolation, minimum paths...) have been more extensively studied and are more familiar in the scalar case. The term ‘scalar’ refers to the transport of a scalar quantity (current) as opposed to a vectorial one (force) in mechanical problems. Currents entering one node by the conducting bonds of the network should balance the external current

fed into that node, just like bond forces balance external efforts. The analog of the displacement vector (which, in the general case, also involves angular displacements) is the (scalar) potential of a node, and the duality between forces and displacements translates into the duality between currents and potentials. All the developments of section II, adapted within the ASD to displacements instead of velocities, are valid for resistor networks. δu_l is the potential drop in bond l . One may define spaces $\mathcal{F}, \mathcal{C}, \mathcal{V}, \mathcal{S}_0, M$ operators G and G^T , state the theorem of virtual power, etc... The analog of a system of self-balanced bond forces is a set of currents satisfying the conservation law without any external source, *i.e.*, a combination of current loops. One may define as many linearly independent elements of M as there are disconnected parts in the network. The number of degrees of freedom N_f is now equal to the number of nodes. It is related to the number of bonds N , the number of independent loops h and the number of disconnected parts (1 for a connex network) k by the scalar version of eqn. 16:

$$N + k = N_f + h,$$

a simple topological identity valid for an arbitrary graph.

VI. THE ISOSTATICITY PROPERTY.

A. Statement and context.

We consider an assembly of rigid, frictionless grains that only exert normal contact forces on one another. Those forces might however, be attractive or repulsive. We assume that the system, submitted to a prescribed load, has evolved to an equilibrium configuration in which the contact structure supports the load. We also regard the geometric definition of particles as incompletely known, thereby introducing randomness: such parameters as grain diameters or radii of curvature are to be regarded as distributed over small intervals.

Then one can state the following remarkable property: *with probability one, the problem, posed on the contact structure, is isostatic.*

Such an isostaticity property was (more or less explicitly) reported in ref. [20] and articles cited therein, in the case of triangular lattice systems, within the ASD, with grains satisfying the Signorini condition 21. Isostaticity was also stated in refs. [9, 15, 17, 30], that deal with the same model. Moukarzel [33, 34] then argued that systems of frictionless grains interacting by repulsive elastic contact forces should become isostatic in the limit of large contact stiffnesses. And ultimately, Tkachenko and Witten [35] derived an isostaticity property for disordered systems of rigid frictionless spheres in arbitrary dimension, each grain being submitted to an external force (*e.g.*, to its weight), whatever the sign of contact forces.

Here, we will establish the isostaticity of the *problem* ($h = 0$), rather than the isostaticity of the structure

($h = 0$ and $k = k_0$), in quite general situations. As we shall see in section VIII, full rigidity ($k = k_0$) in addition to absence of hyperstaticity ($h = 0$), is a less general property, of *geometric*, as opposed to *topological*, origin.

B. General arguments.

The arguments we give below to establish the isostaticity property emphasize the peculiarity of equilibrium states, in which sufficiently many intergranular contacts should be created in order to resist the externally imposed forces. Thus such states belong to a subset of configuration space of vanishing measure. Grains have been brought to rest by some unspecified dynamic dissipative process. Our derivation admittedly retains a heuristic flavor, for a definitive proof would require much more specific mathematical assumptions. Readers that demand more mathematical rigour will have realized that arguments presented by other authors [33, 34, 35] are not without reproach either, and may refer to the next paragraph. There, within the ASD (and thus at the expense of additional assumptions about the magnitude of displacements from a reference configuration), isostaticity is rigourously deduced.

To ease the presentation of our arguments, let us introduce a few compact notations. We denote as $(q_i)_{1 \leq i \leq N_f}$ a set of coordinates in configuration space \mathcal{E} . The geometry of the grains depends on some random parameters (sizes, shapes...), collectively denoted as ζ . ζ might be regarded as a vector with a large number, say p , of components: $\zeta \in \mathbb{R}^p$. The evolution of the granular system can be modelled as a function Φ that maps an initial configuration $(q_i)_{1 \leq i \leq N_f}^{(0)}$ to the actual equilibrium configuration $(q_i)_{1 \leq i \leq N_f}$. The motion of the grains from $(q_i)_{1 \leq i \leq N_f}^{(0)}$ to $(q_i)_{1 \leq i \leq N_f}$ might *e.g.*, be described by a differential equation. Φ then expresses the dependence on initial conditions. Φ also depends on ζ , which has the role of a set of parameters. To proceed, one has to assume that this dependence is sufficiently regular: $\Phi : \mathcal{E} \times \mathbb{R}^p \rightarrow \mathcal{E}$ is generally a smooth function. Although the evolution of a pack of grains is expected to exhibit a high sensitivity to parameters and initial conditions, it is dissipative and will bring the system very close to equilibrium in a finite time. Chaotic trajectories deviate fast from one another, but the evolution in a finite time is expected to be expressed by a smooth mapping, that also depends continuously on parameters ζ , except perhaps for peculiar values that correspond to bifurcations between different sets of final states or ‘attraction basins’. If, for instance, one reproduces the same dynamical evolution from the initial to the final configurations and gradually change the size of one particle, one expects, physically, the final state to change only gradually, until for some value of the geometrical change some rearrangement of finite extent will suddenly take place. We assume such bifurcations only occur for isolated values of the parameters, such

that around the actual $\zeta \in \mathbb{R}^p$, there exists generically a neighbourhood Ω within which the parameter set might vary without creating any discontinuity or closing any additional contact in final configuration $(q_i)_{1 \leq i \leq N_f} \in \mathcal{E}$.

Consider now the set L of intergranular contacts corresponding to this configuration (the contact structure, as defined in section II). As ζ changes within Ω , maintained contacts form some non-empty subset of L , which is sufficient to carry the load.

If $\zeta \in \Omega$ varies along a curve parametrized by u , so does, via the mapping Φ , $(q_i)_{1 \leq i \leq N_f}$ in \mathcal{E} . If a contact $(i, j) \in L$ is to be maintained in this motion, one must have:

$$\frac{dh_{ij}}{du} = 0. \quad (30)$$

This means that the coordinates of grains i and j have to adjust to the change in grain geometry ζ . If parameter u is formally regarded as *time*, relative normal velocities $\delta V_{ij} = -\frac{dh_{ij}}{du}$, in all contacts that are maintained, are required to balance the effect of the change of ζ , to ensure that equality 30 is still satisfied. Increasing, if needed, the number p of ζ components, it is natural to assume that such conditions on relative velocities are independent from contact to contact, for the required value of δV_{ij} only depends on those geometric parameters that govern the shape of grains i and j in the immediate vicinity of their contact point. Therefore, for a list L of N contacts to be maintained for arbitrary $\zeta \in \Omega$, any N -vector $(\delta V_l)_{1 \leq l \leq N} \in \mathbb{R}^N$ of possible relative normal velocities in the contacts of L must be compatible. In view of condition 15, only such contact structures L that are devoid of self-balanced sets of internal forces (*i.e.*, such that $h = 0$ or $\mathcal{S}_0 = \{0\}$) can be maintained. If, exceptionnally, the equilibrium configuration $(q_i)_{1 \leq i \leq N_f}$ admits one non-vanishing element $(\gamma_l)_{1 \leq l \leq N}$ of \mathcal{S}_0 , then, as the condition

$$\sum_{1 \leq l \leq N} \gamma_l \delta V_l = 0$$

cannot be ensured for arbitrary $(\delta V_l)_{1 \leq l \leq N} \in \mathbb{R}^N$, and grains cannot interpenetrate, one at least of the contacts l such that $\gamma_l \neq 0$ will open ($\delta V_l < 0$) upon slightly tampering with geometric parameters ζ .

We have thus shown that, with probability one, the contact structure in the equilibrium configuration cannot be hyperstatic, the degree of indeterminacy of forces h is equal to zero.

The above derivation relies on rather specific assumptions about mapping Φ . One should be aware, however, that we are free to choose any initial configuration that does not violate impenetrability conditions. The assumptions we have relied upon are quite natural when the initial and final equilibrium configurations are close to each other. Basically, one has then to accept the idea that the fine geometrical details of grain surfaces, in the vicinity of their contact points at equilibrium, do not significantly

influence their trajectories except in the very final stage. Thus they can be regarded as randomly chosen during this ultimate stage of the approach to equilibrium, as though the system ‘realized’ then what their actual values are. In the next subsection it is assumed that the ‘initial’ and final state are so close that the motion between them might correctly be described within the ASD. Other derivations might resort to fictitious construction processes of the granular assembly, in which Φ is replaced by a simpler function. One might consider, *e.g.*, sequentially bringing the grains, one by one, to their equilibrium position, thus gradually enlarging the list of contacts. If, at any stage in the process, h is strictly positive, some of the contacts cannot be maintained on slightly altering some of the geometrical details of grain surfaces near the most recently created contacts.

The equilibrium state, as we have just concluded, is devoid of hyperstaticity ($h = 0$). What about its possible mechanisms? We have assumed that it can support the load. It is tempting to conclude that mechanisms do not exist in the generic case, since the orthogonality condition 17 would have to be maintained as the shape of the grains is altered. However, one has to keep in mind that equilibrium configurations are very peculiar ones, and we shall see that the existence of mechanisms in the equilibrium state depends in general on the sign of intergranular forces, and on the shape of the grains.

C. Alternative derivation within the ASD. The special case of lattice models.

A slightly different point of view may be adopted in the framework of the ASD: within the approximation, the problem being replaced by a simplified one, the isostaticity property can be established in a rigorous way. Also, the analogy with the scalar problem might make the result more immediately intuitive. Let us assume the ASD to be valid with a reference configuration in which all contacts are slightly open: a list of bonds is defined, with strictly positive values of interstitial thicknesses h_l^0 . h_{ij}^0 , the distance separating the surfaces of grains i and j is to be regarded as a random number that depends on fine details of their geometry. h_{ij}^0 values for the different bonds are independent and continuously distributed. Once the system has been brought to an equilibrium configuration, forces are carried by contacts, *i.e.* bonds l for which $h_l = 0$. If $(\gamma_l)_{1 \leq l \leq N}$ is a set of self-balanced forces carried by those contacts, the theorem of virtual work, applied with such bond forces on the one hand, and with the displacements from the reference to the equilibrium configurations on the other hand, yields :

$$\sum_{l=1}^N \gamma_l (h_l^0 - h_l) = \sum_{l=1}^N \gamma_l h_l^0 = 0. \quad (31)$$

Thus a certain linear combination of the random distances h_l^0 has to be equal to zero. Coefficients $(\gamma_l)_{1 \leq l \leq N}$

are fixed once the reference configuration is known. Moreover, *via* an iterative dilution process, they can be chosen among a finite set, as we now show: assume a set of self-balanced forces $(\gamma_l)_{1 \leq l \leq N}$ to exist, and define the set B_0 of bonds l for which $\gamma_l \neq 0$. Then, as long as it is possible, proceed to successive ‘dilutions’ of this set, defining B_1, B_2, \dots requesting that there is one bond less in B_{k+1} than in B_k , but that it is still possible to find self-balanced forces localized on the bonds of the reduced set. The final B_{k_0} , that can no longer be diluted, will be such that the values of γ_l will be uniquely determined for each $l \in B_{k_0}$, up to a common factor, which is fixed if one imposes the condition that the largest γ_l is equal to one. In this way, one thus defines *irreducible sets of self-balanced forces*, that are put in one-to-one correspondence with certain substructures of the whole contact structure. In a finite system, one thus has a finite number of such irreducible sets of bond forces. If a system of self-balanced forces can be carried by the contacts that are closed, then equation 31 has to be satisfied with one of the irreducible systems of self-balanced forces, an occurrence of probability zero.

The scalar analog of this derivation is especially straightforward. To the requirement that only particles in contact exert a force on one another corresponds the condition that a bond between sites a and b on the resistor network can only carry a current when the potential difference $v_a - v_b$ is equal to a prescribed value, v_{ab}^0 . Parameters v_{ab}^0 are to be regarded as random, chosen according to a continuous probability distribution and independent from bond to bond. Then, the appearance, once some current is injected at one node of the resistor network and extracted at another, of a loop of current-carrying bonds is to be discarded as an occurrence of zero probability. (One may of course define irreducible loops, as the ones that carry a unit current and do not contain strictly smaller subloops). Assume three bonds, making a loop between three sites, say $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$, to carry a non-vanishing current (figure 8). This implies an exact

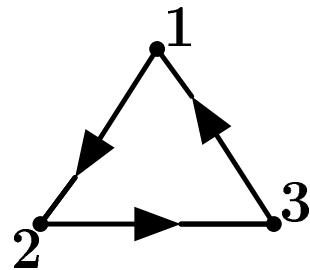


FIG. 8: Three bonds forming a loop in the resistor network. A current might circulate as indicated by the arrows.

relation of the form $\pm v_{1,2}^0 \pm v_{2,3}^0 \pm v_{3,1}^0 = 0$, which has no chance to be satisfied.

Let us consider now, as an example, returning to granular systems, the small hyperstatic structure of fig. 5, and

assume the 7 grains have been brought, from the reference configuration of the triangular lattice model defined in section IVB, in which all interstices are open ($h_{ij}^0 > 0$), to an equilibrium configuration in which the 12 bonds are closed contacts, with $h_{ij} = 0$. Labelling the grains as on the figure, equation 31 reads:

$$\sum_{i=2}^7 h_{1,i}^0 - \sum_{i=2}^6 h_{i,i+1}^0,$$

which is true with probability zero for continuously distributed independent random numbers h_{ij}^0 . Within the lattice model with random diameters, as introduced in section IVB, one has

$$h_{ij}^0 = \frac{a}{2}(\delta_i + \delta_j)\alpha, \quad (32)$$

one obtains a relationship between δ_i 's:

$$\delta_1 = \frac{1}{6}(\delta_2 + \delta_3 + \delta_4 + \delta_5 + \delta_6 + \delta_7),$$

which, once again, is satisfied with probability zero.

It is less obvious, however, that the disorder on the radii of discs that remain exactly circular (or of perfect spheres in 3D) is sufficient, because of the induced disorder on h_{ij} 's, as in eqn. 32, to forbid the existence of *any* set of self-balanced contact forces. The problem is that, because of 32, interstitial thicknesses are no longer independent. On transforming 31 into a relation between δ_i 's, one gets

$$\sum_i \left(\sum_{j \neq i} \gamma_{ij} \right) \delta_i = 0,$$

which might well be satisfied if $\sum_{j \neq i} \gamma_{ij} = 0$ for each i . This latter condition has no chance to be obeyed in a disordered system, but may be achieved on a regular lattice. This does not occur, however, with nearly monodisperse discs on the regular triangular lattice in 2D, because 3 independent conditions per disc are to be satisfied, and the number of contacts, at most three times the number of discs on this 6-coordinated lattice, has to be strictly smaller, because hyperstatic configurations like that of fig. 5 cannot exist.

The situation is different for the analogous 3D model, defined with slightly polydisperse spheres on the sites of an FCC lattice. Each sphere has 12 nearest neighbours, and one may find hyperstatic structures in which contacts will be maintained with polydisperse spheres. A simple example of such a structure can be found, with 24 spheres and 64 contacts[60]. Although a small amount of polydispersity eliminates hyperstaticity in 2D triangular lattices of discs, it does not do so in FCC lattices of spheres, provided the grains, in spite of the distribution of radii, remain perfectly spherical. If the shape of the grains is also affected by the slight geometric disorder, then (with the notations of fig. 4), one has $\|\mathbf{R}_{ij}\| \neq \|\mathbf{R}_{ik}\|$

for $j \neq k$, interstitial thicknesses h_{ij} become independent in all bonds of the lattice, and hyperstaticity is forbidden. (Within the ASD, it is consistent to ignore the rotation of unit vectors \mathbf{n}_{ij} due to small departures from sphericity).

D. Consequences. Remarks.

Once the list of active contacts in an equilibrium state is known, isostaticity of the problem enables a purely geometric determination of the forces, independently of material properties. As an example, system C was brought in equilibrium under the load defined by eqn. 19, with conditions 21. As soon as the list of contacts (structure SC) is known, the set of normal contact forces is entirely determined.

This gives a meaning to the limit of rigid particles: in generic situations, when the sizes and shapes of the grains are affected by some amount of randomness, there is no problem of force indeterminacy once an equilibrium configuration has been reached. The actual value of contact forces will not depend on the detail of the contact law, provided it might be regarded as rigid, but it will be sensitive to fine geometrical details. As an example, consider frictionless elastic contacts obeying eqn. 26. Let us assume a stable equilibrium state of the grain assembly, regarding the grains as perfectly rigid (condition 21), has been reached. One thus has a local minimum of W (defined in eqns. 4 or 5). Then, let us take into account the finite, but small, deformability of the contacts. The same list of contacts will carry forces that, to first order in the small displacements, do not change. Evaluation, within the ASD, of relative normal displacements $h_l < 0$ in force carrying contacts yields $h_l = -(\frac{f_l}{K_l})^{1/m}$, such relative displacements are compatible because of the isostaticity property, and the resulting elastic energy,

$$W^{el} = \frac{1}{m+1} \sum K_l |h_l|^{m+1} = \frac{1}{m+1} \sum K_l^{-1/m} f_l^{(m+1)/m},$$

tends to zero as stiffness constants K_l tend to infinity. Thus the actual values of constants K_l and exponent m (these data might vary from contact to contact) are irrelevant.

Once an equilibrium state has been reached, force values do not depend on the details of the contact law: this is an important step on the way to the *reduction of the mechanics of granular systems to geometry*—the basic goal of the present paper. This contributes to ease the derivation of generic mechanical properties of granular systems.

The simplification that results from the isostaticity property should however be balanced with the two following difficulties.

Firstly, configurations of granular systems, due to the same isostaticity property, are necessarily quite sensitive to fine geometric details: tiny variations of grain dimensions or positions might lead to opening of some contacts. As all contacts are indispensable to support the load, the system has to rearrange somehow to create other contacts

that compensate for one that were lost. This is the origin of a property known as *fragility*, to be more accurately defined, and discussed, in part IX.

Secondly, one should be aware that the choice of an equilibrium configuration among several possible ones might depend on other physical parameters than the geometry of the grains. The reduction to geometry is thus not complete. In section VII below, the consequences of the ASD are studied, and it is shown that mechanical problems are entirely geometric within the approximation.

As a consequence of the absence of hyperstaticity ($h = 0$), one readily obtains, from 16, a bound on the number of contacts N that carry a force, involving the number N_f of degrees of freedom of the particles belonging to the backbone of the force-carrying structure: $N \leq N_f - k_0$. Neglecting the effect of boundary conditions on the count of N_f in large granular systems, one gets an upper bound on the coordination number $c = \frac{2N}{n}$:

$$\begin{cases} c \leq 2d & \text{for spheres} \\ c \leq d(d+1) & \text{in the general case,} \end{cases} \quad (33)$$

Particles in 3D that possess an axis of revolution, like spheroids, also have one trivial rotational free motion (in the absence of friction). Thus one should subtract one degree of freedom for each, hence the bound $c \leq 10$, instead of the general 3D value 12.

Interestingly, an estimate $c \simeq 11$ for the coordination number of long rods or fibers was given by Philipse [36], on the basis of some statistical assumptions about the random packings of such particles.

What we have established is in fact the *absence of hyperstaticity of a generically disordered assembly of rigid grains, regarded as frictionless*. Forces, in the derivation, only appear as convenient auxiliary quantities ('virtual' forces) to deal with a purely geometric problem. The conclusions thus holds in the presence of solid friction. Assemblies of rigid grains with friction therefore abide by inequality 33. (It is of course well known, from numerical simulations in particular [37, 38, 39], that the contact coordination number is a decreasing function of the friction coefficient).

It is also worth pointing out that 33 does not depend on the polydispersity of the grains. Grains that are much larger than their neighbours will often touch a large number of them. However, this effect should be compensated in the average coordination number by an opposite one, affecting small grains. When they touch a large one, this latter effectively occupies half of the surrounding space, thereby reducing the possibility for other contacts.

On the ground that force-carrying structures should be rigid (devoid of mechanisms, $k = k_0$) the *opposite* inequality, $N \geq N_f$, whence the *lower* bound $d(d+1)$ ($2d$ for spheres or discs) for the coordination number, is sometimes quoted in the literature [35, 40]. We regard it as wrong in general (although true for systems of non-cohesive rigid frictionless spheres, as we shall see). As pointed out by Alexander [40], the physically relevant

concept is not rigidity, but stability (under a given external load). This is discussed in section VIII below. First, section VII is devoted to the exploitation of potential minimization properties within the ASD.

VII. EQUILIBRIUM AND POTENTIAL MINIMIZATION WITHIN THE ASD.

The approximation of small displacements introduced in section IV has several important consequences. Finding an equilibrium state amounts, in some cases, to solving a convex minimization problem, for which optimization theory provides useful properties and tools. The relationship with percolation or minimum path models are also to be discussed within the ASD.

A. Convexity.

When the potential energy is a convex function of displacements or positions, and when the rigid constraints define a convex set in configuration space, then the search for a stable equilibrium state is a convex optimization problem, and the following important properties can be exploited [41].

1. The equilibrium conditions, which express the *stationarity* of the potential, are not only *necessary* conditions for potential minimization (*i.e.*, stability), they are also *sufficient*.
2. A local minimum of potential W is a global minimum. W is flat, equal to its minimum value, over a convex set of possible equilibrium configurations.
3. A structure being given, a supportable load will be supported.
4. Equilibrium forces are the solution to another optimization problem (the so-called *dual problem*).
5. Rigid laws and elastic ones can be dealt with in the same way.

Let us, among the contact laws presented in section III, distinguish the ones that lead to convex problems. It should be remarked first that standard convexity is defined in vector spaces, not on manifolds. In order to exploit the classical results of convex optimization theory to grains of arbitrary shape, it is necessary to place ourselves within the frame of the ASD, which replaces the curved configuration space by its flat tangent space \mathbb{R}^{N_f} .

As intergranular distances h_l are, within the ASD, affine functions of displacements, it follows that both rigid constraints $h_l \geq 0$ or $h_l \leq 0$ define a convex set (and so does $h_l = 0$): the accessible part of configuration space is a simplex, a convex set whose boundaries are a collection of flat sections (parts of affine spaces). Since

the potential energy of external forces, W , is linear in the displacements, its minimization belongs to the class of *linear optimization problems*, that are the subject of a large literature in applied mathematics and operational research. This important case –granular systems within the ASD with contact laws of type 21, or systems abiding by 23 or 24 , or tensegrities–is dealt with in detail in section VIIIB.

Still within the ASD, contact laws involving smooth interaction potentials will lead to convex problems if the potential function w is convex. This is the case for unilateral elasticity, as defined in 26 and 27, but not for intergranular potentials that possess an attractive tail like on figure 7.

Outside the ASD, convexity can be discussed in the case of spheres or discs, since, ignoring rotations, their configuration space is flat. One immediately checks, then, that impenetrability constraints $h_l \geq 0$, once h_l is no longer approximated as an affine function of displacements, define a non-convex set of admissible configurations. The opposite inequality $h_l \leq 0$, on the contrary, does lead to convex problems. As we shall see, frictionless spheres on the one hand, and systems of strings tied together on the other hand behave exactly in the same way, upon reversing the sign of forces and deformations, *within* the ASD, but strongly differ *without* the ASD.

B. Rigid, unilateral contact law.

1. Context. Notations

The properties of convex problems enumerated above are valid, in particular, in the case of linear optimization problems, for which they are sometimes presented in particular forms [41, 42]. Here, in order to stress their physical meaning, we shall directly rederive them. We consider an assembly of rigid frictionless grains, satisfying the Signorini conditions 21, dealt with within the ASD. We assume a structure has been defined, and if the load is supported, some of its N bonds will, at equilibrium, close ($h_l = 0$) and transmit a force ($f_l > 0$). The following also applies if condition 21 is replaced by 23 or 24.

Keeping the same notations as in sections II and IV, we know that the impenetrability constraints are expressed with matrix G

$$\text{For } 1 \leq l \leq N, \quad \sum_{\mu=1}^{N_f} G_{l\mu} u_\mu \leq h_l^0, \quad (34)$$

the transpose of which appears in the equilibrium equations

$$\text{For } 1 \leq \mu \leq N_f, \quad \sum_{l=1}^N G_{l\mu} f_l = F_\mu^{ext}. \quad (35)$$

Throughout this section, compact notations will be used for vectors of external forces (\mathbf{F}^{ext} for $(F_\mu^{ext})_{1 \leq \mu \leq N_f}$) contact forces (\mathbf{f} for $(f_l)_{1 \leq l \leq N}$), interstices (\mathbf{h} for $(h_l)_{1 \leq l \leq N}$), and displacements (\mathbf{u} for $(u_\mu)_{1 \leq \mu \leq N_f}$), the bracket notation (*e.g.*, $(\mathbf{f}|\mathbf{h})$) is used for scalar products, while operator notations and abbreviation for inequalities reduce 34 to $G\mathbf{u} \leq \mathbf{h}^0$.

2. Minimization in displacement space.

We now show that finding equilibrium displacements is *equivalent* to solving the following linear optimization problem:

$$\mathcal{P}_1 \left\{ \begin{array}{l} \text{Minimize } W = -Q\lambda = -\sum F_\mu^{ext} u_\mu \\ \text{with constraints: (34)} \end{array} \right.$$

We know from section III that a solution to problem \mathcal{P}_1 provides a set of Lagrange parameters $(f_l)_{1 \leq l \leq N}$ that satisfy both conditions 21 and 35 (or 22), and are therefore equilibrium forces.

Conversely, in the case of a linear optimization problem such as \mathcal{P}_1 , the stationarity condition is sufficient to ensure that W is minimized.

This can be checked as follows: let $\mathbf{u}^* \in \mathcal{V}$ represent one solution for displacements, and, likewise, let us denote equilibrium contact forces as $\mathbf{f}^* \in \mathbb{R}^N$. To \mathbf{u}^* corresponds the set of values \mathbf{h}^* for interstitial distances, and the Signorini condition might be expressed as

$$(\mathbf{f}^*|\mathbf{h}^*) = 0,$$

while any displacement vector $\mathbf{u} \in \mathcal{V}$, corresponding to \mathbf{h} , satisfies

$$(\mathbf{f}^*|\mathbf{h}) \geq 0.$$

From the theorem of virtual work, one then has

$$W(\mathbf{u}) - W(\mathbf{u}^*) = -(\mathbf{f}^*|\mathbf{h}^*) + (\mathbf{f}^*|\mathbf{h}) \geq 0$$

and displacement \mathbf{u}^* minimizes the potential energy.

Figure 9 is a schematic representation of problem \mathcal{P}_1 . A simplex, defined by a set of affine constraints like 34, is limited by flat faces, where some of the constraints are active. Its extreme points (the ‘corners’) are where a maximum list of constraints are simultaneously active. The criterion to be minimized is itself an affine function, it is constant on hyperplanes that are orthogonal to the load. Equilibrium is achieved on the simplex boundary, at least in one extreme point, in general on a simplex A in a space that is orthogonal to the load direction. Let k (smaller than N_f) denote the dimension of this space. Within the set of solutions, W is constant, and a certain number N^* of contacts are maintained closed. Let us denote this structure as S^* : it is the list of contacts that are closed for all equilibrium configurations. For those equilibrium states that are on the boundary of A , some additional contacts are created. It follows from its

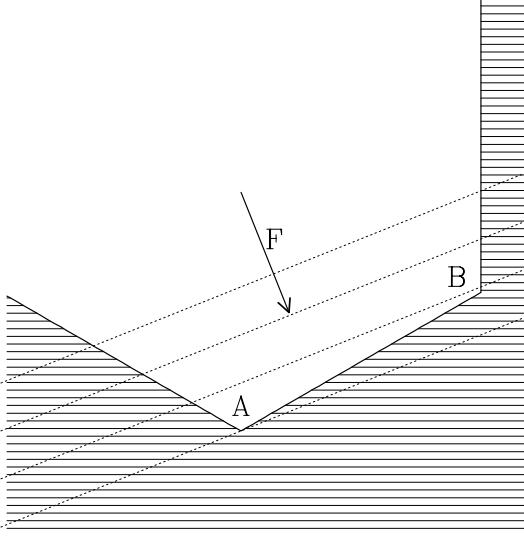


FIG. 9: Aspect of simplex of variables satisfying affine constraints like 34, cut by the plane of the figure. W is constant on parallel hyperplanes (sketched as dotted lines, orthogonal to F , projection of load direction onto the plane). W reaches its minimum at one extreme point at least (like A and B) or on ‘faces’ or ‘edges’, included in an affine space of dimension k , that are part of the simplex boundary, (like segment AB). The hatched region is forbidden by impenetrability constraints.

definition that k is the degree of velocity (here, within the ASD, of displacement) indeterminacy of S^* . Since, from part VI, its degree of hyperstaticity is zero, one has $k = N_f - N^*$.

3. Supportable loads will be supported.

In general, displacements are thus determined up to some motion within convex set A .

Let us now show that A is not empty if the load is supportable. We assume some statically admissible forces $(f_l^0)_{1 \leq l \leq N}$ to be defined on the bonds of the complete structure that was defined a-priori. Then a finite lower bound for W on the whole simplex of admissible displacements can be obtained upon writing the variation of W from the reference configuration as

$$\Delta W = - \sum_{1 \leq l \leq N} f_l^0 \delta u_l \geq - \sum_{1 \leq l \leq N} f_l^0 h_l^0.$$

W , thus, cannot decrease to $-\infty$ within the simplex, and has to reach a finite minimum somewhere on the boundary. Moreover, one can show that A is also bounded, except for *marginally* supportable loads. We say the load is *not* marginally supportable if there exists a small neighbourhood of $(F_\mu^{ext})_{1 \leq \mu \leq N_f}$ in force space \mathcal{F} within which all loads are supportable. Let us now consider

a situation in which A is not bounded. One can then find one direction along which displacements go to infinity within A . Now let us assume the load is not marginally supportable. One can apply a small load increment $(\delta F_\mu^{ext})_{1 \leq \mu \leq N_f}$, such that $(F_\mu^{ext} + \delta F_\mu^{ext})_{1 \leq \mu \leq N_f}$ is still supportable, with $(\delta F_\mu^{ext})_{1 \leq \mu \leq N_f}$ in the direction for which A is not bounded, which leads to a contradiction. Therefore the load has to be marginally supportable if A is not bounded.

4. Dual problem in bond force space

We now turn to the dual optimization problem, to which equilibrium contact forces are the solution, *viz.*

$$\mathcal{P}_2 \left\{ \begin{array}{l} \text{Maximize } Z(\mathbf{f}) = -(\mathbf{f}|\mathbf{h}^0) = -\sum_l h_l^0 f_l \\ \text{with constraints: (35) and } \mathbf{f} \geq \mathbf{0} \end{array} \right. \quad (36)$$

We know that equilibrium displacements (\mathbf{u}^*) and contact forces $(\mathbf{f}^* \geq \mathbf{0})$ respectively satisfy 34 and 35, and are such that

$$(\mathbf{f}^* | (G \cdot \mathbf{u}^* - \mathbf{h}^0)) = 0. \quad (37)$$

Thus, any possible set of non-negative bond forces \mathbf{f} balancing the load is such that

$$(\mathbf{f} | (G \cdot \mathbf{u}^* - \mathbf{h}^0)) \leq 0 = (\mathbf{f}^* | (G \cdot \mathbf{u}^* - \mathbf{h}^0))$$

on the one hand, and

$$(\mathbf{f} | G \cdot \mathbf{u}^*) = (G^T \mathbf{f} | \mathbf{u}^*) = (\mathbf{F}^{ext} | \mathbf{u}^*)$$

on the other, which entails $Z(\mathbf{f}) \leq Z(\mathbf{f}^*)$: \mathbf{f}^* is a solution to problem \mathcal{P}_2 .

Conversely, if one starts from problem \mathcal{P}_2 , and consider a solution \mathbf{f}^* , then it is possible to define an N_f -vector \mathbf{u}^* of Lagrange parameters corresponding to constraints 35, and an N -vector \mathbf{h} of non-negative Lagrange parameters corresponding to constraints $\mathbf{f} \geq \mathbf{0}$, such that

$$-\mathbf{h}^0 + G \mathbf{u}^* + \mathbf{h} = 0. \quad (38)$$

Moreover, h_l vanishes whenever $f_l > 0$. This means that \mathbf{u}^* is actually a displacement vector abiding by 34, and equation 38 entails that the Signorini condition, in the form 37, is also satisfied. We know then that \mathbf{u}^* is a solution to \mathcal{P}_1 .

Equilibrium displacements and contact forces thus coincide with the respective solutions to \mathcal{P}_1 and \mathcal{P}_2 , a pair of *linear optimization problems in duality*. We have shown that:

- If \mathbf{u}^* is a solution to \mathcal{P}_1 , then it is possible to find a solution \mathbf{f}^* to \mathcal{P}_2 , 37 being satisfied.
- If \mathbf{f}^* is a solution to \mathcal{P}_2 , then it is possible to find a solution \mathbf{u}^* to \mathcal{P}_1 , 37 being satisfied.

- If \mathbf{u}^* and \mathbf{f}^* respectively abide by the constraints of optimization problems \mathcal{P}_1 and \mathcal{P}_2 , and if, in addition, 37 (equivalent to the Signorini condition 21) is satisfied, then \mathbf{u}^* and \mathbf{f}^* are respectively solutions to \mathcal{P}_1 and \mathcal{P}_2 .
- The optimum value of the criteria are equal in both problems: condition 37 ensures $W(\mathbf{u}^*) = Z(\mathbf{f}^*)$.

5. The uniqueness property.

Within the affine space of bond forces satisfying 35, constraints $f_l \geq 0$ define a simplex, and, just like for \mathcal{P}_1 , the set of solutions to \mathcal{P}_2 is a convex part B of its boundary. Let h denote the dimension of the affine space spanned by B . Since B is the set of possible equilibrium forces, h is in fact the degree of force indeterminacy of the problem. Generically, one has, from part VI, $h = 0$, and the only solution to problem \mathcal{P}_2 is an extreme point of the simplex of admissible forces. We have thus shown that *in terms of forces, the solution is uniquely determined*. This is a stronger conclusion than the sole isostaticity of the problem established in part VI: in general, contact forces are uniquely determined *once the list of contacts is known*. In the case of a system of rigid grains, with contact law 21, dealt with within the ASD, *the list of force-carrying contacts itself* (the list of bonds, among those that are defined a-priori in the reference configuration, for which neighbouring grains will actually touch and exert a force on each other) *is uniquely determined*. Forces are carried by contact structure S^* , which was defined in connection with the discussion of the solutions to problem \mathcal{P}_1 , and, if some mechanisms exist ($k > 0$), the other contacts that might be created will not carry any force.

If the contact law is 21, if geometrical changes from a reference configuration are small enough for the ASD to be valid, if the load is supportable (but not marginally so), then the system will reach an equilibrium state, which apart from bounded displacements within convex set A (that do not change W) is totally independent of all dynamical properties of the system, and entirely determined by the sole geometry.

6. Examples.

Systems A and B introduced in part II, were treated within the lattice model defined in section IV.B, with the ASD, and condition 21. Structure SA1, once the random numbers δ_i were known, was obtained as the uniquely determined list of force-carrying contacts at equilibrium under the load defined by 18. Within the ASD, it is possible to close 2 other contacts, *e.g.*, those that belong to SA2. However, they will not transmit any force. Likewise, for specific values of the δ_i 's, SB1 was obtained as the list of force-carrying contacts in system B submitted

to the load that is represented on figure 2. It is possible to close some other contacts (such as those that belong to SB2), but they cannot carry (within the ASD) any force. Uniquely determined force-carrying structures, depending on the load, will possess a varying degree of displacement indeterminacy k . Once system B, in addition to the forces on the perimeter, was submitted to small (randomly oriented) external forces exerted on each grain, then isostatic structure SB2 was obtained.

In ref. [9], the triangular lattice model, as in section IV.B, was studied for isotropic loads. As an application of the *global* minimization property, it was shown, within the ASD (to first order in α) that *the maximum packing fraction of polydisperse discs is, in the limit of large systems, equal to*

$$\Phi_{max} = \frac{\pi}{2\sqrt{3}}(1 - k\alpha), \quad (39)$$

with $k = 0.314 \pm 0.003$ in the case of a uniform distribution of radii.

7. Minimal structures. Analogies with other problems.

As equilibrium contact forces are the coordinates of an extreme point of the simplex of problem \mathcal{P}_2 , a maximum set of inequality constraints $f_l \geq 0$ are simultaneously satisfied as equalities, $f_l = 0$. This means that force-carrying structure S^* is minimal with respect to the equilibrium requirement 35. In section VI.C, we invoked an iterative dilution process to define irreducible sets of self-balanced forces. Likewise, one can define minimal structures, such as S^* , as irreducible by further dilution, since it is impossible to require more bond forces to vanish if the load is to be balanced. Any such irreducible structure S might carry a unique set of bond forces balancing the load, it geometrically determines one solution to equations 35.

Recalling we have defined a loading parameter Q , to which all external forces are proportional, there exists for each minimal force-carrying structure S a set of coefficients $(\beta_l^S)_{1 \leq l \leq N}$, such that the forces carried by S that balance the load are

$$f_l = \beta_l^S Q. \quad (40)$$

By definition, one has

$$\begin{cases} \beta_l^S \neq 0 & \text{if } l \in S \\ \beta_l^S = 0 & \text{if } l \notin S \end{cases}$$

Among all minimal structures S with non-negative coefficients β_l^S , S^* minimizes

$$\sum_{l \in S} \beta_l^S h_l^0.$$

Let us now recall the analogy with a problem of current transport on a resistor network, as introduced in part V,

with the following constitutive law. To the requirement that contact forces are repulsive corresponds an *orientation* of the bonds, which behave as diodes rather than resistors. Bond $a \rightarrow b$ between nodes a and b carries some current $i_{ab} \geq 0$ that is related to the potential difference $v_a - v_b$ by the analog of the Signorini condition:

$$\begin{cases} i_{ab} > 0 & \text{if } v_a - v_b = v_{ab}^0 \\ i_{ab} = 0 & \text{if } v_a - v_b < v_{ab}^0 \end{cases} \quad (41)$$

The bond becomes a supraconductor (the analog of a rigid contact) when the threshold potential difference v_{ab}^0 is reached, and it is an insulator if $v_a - v_b$ is smaller.

It is customary to define a scalar analog of the mechanical load by injecting some external current I in one node, that we denote as i , and extracting it from another one, that we denote as o . I is then the analog of the mechanical parameter Q . A minimal structure (*i.e.*, one that cannot be further diluted), to carry the current, is a *path* from i to o . If its coefficients β cannot be negative, it is a *directed path*, on which the current flow respects the a-priori orientation of the bonds. On such a path S , all bonds $l \in S$ carry the total current I , hence $\beta_l^S = 1$ for all $l \in S$. In the analogous scalar problem, the current is carried by the directed path S^* that minimizes, among all directed paths S from i to o , the criterion

$$\sum_{l \in S} \beta_l^S v_l^0 = \sum_{l \in S} v_l^0.$$

In the scalar problem, the criterion reduces to a sum of ‘costs’ associated with the bonds of the network.

The analogous problem to \mathcal{P}_2 in the scalar case is thus the well-known *minimum directed path* (or *directed polymer*) problem on a network [43]. This analogy was introduced in [20], for problem \mathcal{P}_1 , upon transforming the minimum path problem into the dual problem, which consists in maximizing the potential drop $v_i - v_o$, knowing that in each bond l v_l cannot exceed the threshold value v_l^0 . The dual point of view adopted here—the analogy for problem \mathcal{P}_2 —stresses the geometric origin of equilibrium forces, as coefficients characterizing the maximum localisation of efforts onto structure S^* . Contact forces in granular packings have often been studied in the recent literature [10, 44, 45]. It is interesting to be able to define them as the solution to a well-defined optimization problem of random geometry [17].

Some statistical properties of structures S^* were studied in refs. [9, 15], in the case of the 2D triangular lattice model, as defined in section IV.B, with a uniform distribution of δ_i ’s. It was shown, in particular, for isotropic loads in the limit of large systems, that the density of force-carrying bonds tends to a non-vanishing limit, and the distribution of contact force values was evaluated.

The statistical properties of the solution to the ‘directed polymer’ problem are related to those of directed percolation [43]. Likewise, one can expect, in the case, in particular, of a very wide distribution of values of h_0 in

the mechanical problem, minimization problem \mathcal{P}_2 to be related to some unilateral percolation problem. Such a percolation model was never studied to our knowledge. It is a *geometric* problem, unlike generic central force percolation [22], for which (in 2D at least) only the topology of a diluted structure matters.

8. Some macroscopic results for the triangular lattice model.

To see what macroscopic mechanical behaviour might result from the properties stated in this section, we briefly recall here some results obtained by numerical simulation of the triangular lattice model [17], as presented in section IV.B, with a uniform distribution of parameters δ_i (eqn. 29).

Samples of up to 12600 discs were submitted to varying states of stress. The following inequalities, in which coordinate label 1 corresponds to one of the three directions of dense rows in the triangular lattice, and compressive stresses are conventionally positive, define the domain of supported loads, as macroscopically expressed in terms of stresses.

$$\begin{cases} \sigma_{22} \leq 3\sigma_{11} \\ -\frac{\sigma_{22}}{\sqrt{3}} \leq \sigma_{12} \leq \frac{\sigma_{22}}{\sqrt{3}} \end{cases} \quad (42)$$

All intensive quantities, like, *e.g.*, distributions of force values, density of the contact structure, distribution of contact orientations, etc... were found to possess well-defined thermodynamic limits, independently of the details of the boundary conditions, provided a uniform state of stress is imposed, and the stress tensor $\underline{\underline{\sigma}}$ satisfies conditions 42 as strict inequalities. Correlation lengths or, in other words, sizes of representative volume elements, or of independent subsystems, are finite, but appear to diverge as marginally supported loads (for which one of conditions 42 holds as an equality) are approached.

Taking, as in section IV.3, the undisturbed lattice, in which the spacing between sites is equal to a , the maximum disc diameter, as the reference state, a strain tensor $\underline{\underline{\epsilon}}$ can be identified. It is related to displacement field \mathbf{u} by

$$\epsilon_{\alpha\beta} = -\frac{1}{2} \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right), \quad (43)$$

and the potential energy per unit surface area is (summation over repeated indices implied)

$$W = -\sigma_{\alpha\beta}\epsilon_{\beta\alpha} = -\underline{\underline{\sigma}} : \underline{\underline{\epsilon}}. \quad (44)$$

Coordinates of tensor $\underline{\underline{\epsilon}}$ are found to be expressible as linear combination of the average of bond elongations δu_l for the three bond orientations of the triangular lattice. In $\underline{\underline{\epsilon}}$ space (3-dimensional for a 2D system), impenetrability conditions define, in the thermodynamic limit, a

strictly convex accessible domain \mathcal{D} , limited by a smooth surface Σ , the equation of which we denote as

$$f(\underline{\epsilon}) = 0, \quad (45)$$

while the interior of accessible region \mathcal{D} corresponds to the strict inequality:

$$f(\underline{\epsilon}) < 0.$$

As a macroscopic consequence of the variational properties stated in part VII, the relationship between tensors $\underline{\sigma}$ and $\underline{\epsilon}$ is the following:

$$\begin{aligned} \sigma_{ij} &= \lambda \frac{\partial f}{\partial \epsilon_{ij}}, \text{ with } \lambda \geq 0, \text{ if } f(\underline{\epsilon}) = 0 \\ \sigma_{ij} &= 0 \quad \text{if} \quad f(\underline{\epsilon}) < 0 \end{aligned} \quad (46)$$

Wherever the granular system transmits stress, the value of $\underline{\epsilon}$ is as far as possible in the direction of $\underline{\sigma}$ within \mathcal{D} , i.e., where the tangent plane to its boundary Σ is orthogonal to $\underline{\sigma}$, thus minimizing potential energy 44.

$\bar{\mathcal{D}}$ is unbounded in the direction of non-supported loads. Strains go to infinity on surface Σ when the stress tensor approaches one of the marginally supported directions. Σ has three asymptotic planes, respectively orthogonal to those three marginally supported load directions.

The one-to-one correspondence between supported stress *directions* on the one hand, and strain tensors such that $f(\underline{\epsilon}) = 0$ on the other hand, is a macroscopic translation of the uniqueness property stated in paragraph VIIB5. The potential energy density has a finite thermodynamic limit (a result that generalizes to non-isotropic states of stress the one of equation 39), and possible variations of $\underline{\epsilon}$ within convex set A , discussed in VII.B.3, shrink to a vanishing range ($\underline{\epsilon}$ becomes uniquely determined) as the system size grows.

Constitutive law 46 can be used to solve for stress and displacement fields whenever a sample of the model material is submitted to some external forces that do not lead to unbounded displacements and overall failure. The field of λ values should be obtained on solving the full boundary value problem.

C. Systems with bounded tensile forces.

If the unilateral contact law 21 is replaced by 25, the remarkable properties stated above in VII.B are lost. Let us illustrate this on a simple example. Consider the system depicted on figure 10, to be dealt with, within the ASD, as a triangular lattice model in the sense of IV.B, the contact law being 25. Only one disc is mobile (number 1), and we first consider the case of a vertical force of intensity F_y oriented downwards like on the figure, keeping $F_x = 0$. (Later in part IX we come back to this simple example and discuss its behaviour when F_x is altered). Two equilibrium positions are possible: disc 1

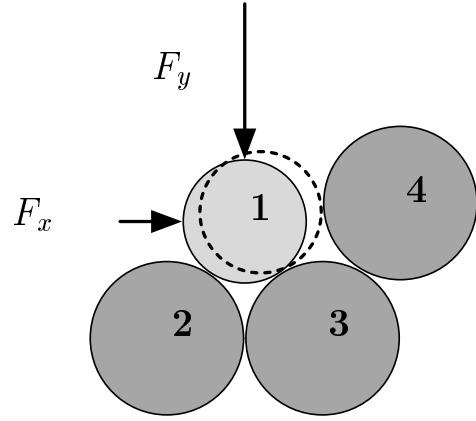


FIG. 10: A small sample of the triangular lattice model, in which the only mobile disc, marked 1, is slightly smaller than discs 2, 3 and 4, and is submitted to an external force. Disc 1 is shown in one possible equilibrium position, in contact with 2 and 3. The other one is sketched with a dotted line.

might either be in contact with discs 2 and 3, or with 3 and 4. As grains are rigid and only exert normal forces on one another when they exactly touch, the problem is isostatic in both equilibrium configurations, in agreement with the general property of section VI. The load, defined with $F_y > 0$, is always supportable on structure S_1 , consisting in bonds 1–2, 1–3, and it is also supportable on structure S_2 , consisting in bonds 1–3, 1–4 as long as $F_y < f_0\sqrt{3}$.

Thus, for $0 < F_y < f_0\sqrt{3}$, even within the ASD, *the equilibrium state and the list of force-carrying contacts are not uniquely determined*. Whether S_1 or S_2 will be chosen depends on the trajectory of disc 1 from its initial (reference) position.

Likewise, *supportable loads are not necessarily supported*. To check this, let us remove disc 2. In its motion, disc 1 might come into contact with both 3 and 4, and, provided $0 < F_y < f_0\sqrt{3}$, reach an equilibrium position, maintaining those two contacts. However, it might as well never meet disc 4, and find a trajectory, past disc 3, on which its potential energy will keep decreasing forever.

D. Smooth, convex interaction potentials.

In the case of the elastic contact law 26, within the ASD, all properties of convex problems enumerated in section VII.A are valid. Let us state the ‘elastic’ versions of the ‘rigid’ optimization problems of VII.B. \mathcal{P}_1 is simply replaced by

$$\mathcal{P}_1^{el} : \text{Minimize } W^{tot} \text{ defined in 28,}$$

while contact forces are the solution to

$$\mathcal{P}_2^{\text{el}} \left\{ \begin{array}{l} \text{Maximize } - \sum_l \left(h_l^0 f_l - \frac{m}{m+1} K^{-1/m} f_l^{(m+1)/m} \right) \\ \text{with constraints: (35) and } \mathbf{f} \geq \mathbf{0} \end{array} \right. \quad (47)$$

The function of contact force f that appears within the sum is the opposite of the Legendre transform of the elastic energy w , regarded as a function of relative displacement δu , i.e., $f \delta u - w(\delta u)$, taken with $f = \frac{dw}{d(\delta u)}$. Thus, solving $\mathcal{P}_2^{\text{el}}$ amounts to ‘minimizing the complementary energy’, a common procedure to find the forces in an elastic problem.

In fact, one could have defined a potential energy, in the rigid case, equal to $+\infty$ if grains interpenetrate, and treat rigid problems exactly like elastic ones, constraint 34 being taken care of by the definition of the potential. If the region, in phase space, that is forbidden by the constraints is convex, then such a potential can still be regarded as a convex function. Both the condition 21 and elastic law 26 are then expressed by

$$f \in \partial w(\delta u),$$

in which $\partial w(\delta u)$ denotes the *subdifferential* of w at δu , i.e., the set of all f such that $w(\delta u') \geq w(\delta u) + f(\delta u' - \delta u)$ for any $\delta u'$. This mathematical possibility to unify rigid and elastic laws is specific to convex problems. This is the precise meaning of property 5 cited in section VII.A. Here, we preferred to resort to a separate presentation of the rigid case in section VII.B, to stress the physical consequences of the variational properties. The reader may refer to [46] for a more systematic approach.

Comparing \mathcal{P}_2 and $\mathcal{P}_2^{\text{el}}$, as defined by 36 and 47, one may expect the following behaviour for the distribution of contact forces, as a set of grains with elastic contacts is submitted to a constant load, but the stiffness constant K is gradually reduced. (Similarly, one could also increase Q , keeping K constant). When K is very large, the elastic term is negligible in comparison with $Z(\mathbf{f})$, and the values of the forces should coincide with the (unique) rigid contact solution of \mathcal{P}_2 . Thus the contact structure should barely suffice to carry the load (isostatic problem), the forces should exhibit the characteristic disorder of granular systems, with large fluctuations, force chains, etc... On the other hand, let us assume that the list of possible contacts (structure S_0) is well-coordinated, that there are many more contacts that are easy to close upon increasing the confining forces or decreasing the contact stiffness parameters. Then, in the limit of small K , $Z(\mathbf{f})$ will, in turn, become small in comparison with the elastic energy. The elastic term tends to share equally the forces between contacts. Thus, a narrow distribution of force values is expected in this limit, and spatial heterogeneities should be strongly reduced. Knowing that the minimum structure S^* and the complete list of possible contacts S_0 are of comparable densities, the order of magnitude of the average force f_0 does not change as grains

are made softer. The two extreme regimes of stiff and soft contacts should thus be respectively defined by the conditions $K \gg \frac{f_0}{h_0^m}$ and $K \ll \frac{f_0}{h_0^m}$, involving a typical interstitial distance h_0 .

Those two limits, and the transition regime, in which the contact density increases, were observed [16] on the 2D triangular lattice model, as defined in section IV.B, with contact law 26.

E. Remarks. The ‘elasticity’ of rigid grains.

As announced beforehand, we have exhibited, in this section, model granular systems for which, at the expense of several assumptions, including the validity of the ASD, mechanical properties are entirely determined by geometry.

We have seen that the distinction between systems made of rigid or deformable grains is not necessarily as important as one might have expected: similar potential energy minimization properties might be stated, the limit of large contact stiffnesses might safely be taken without any singularity (subsection D), and macroscopic stress-strain relationships might be written for some systems of rigid grains, as recalled in paragraph B.8. The difference between the systems such that the search for an equilibrium state is a convex minimization problem (in which case the properties listed in subsection A are satisfied) and the others, such as the example of subsection C, is finally more relevant.

Constitutive law 46 expresses a one-to-one correspondence between the direction of stress tensor $\underline{\underline{\sigma}}$ and strain tensor $\underline{\underline{\epsilon}}$, which is restricted to belong to surface Σ . It is quite similar to a macroscopic elastic law, even though it applies to systems of rigid discs. The response to a supported stress increment will be reversible. If this increment, $\underline{\underline{\delta\sigma}}$ is in the direction of the preexisting stress tensor $\underline{\underline{\sigma}}$, then no additional displacement or stress will result for rigid grains. For deformable grains, if contact law 21 is replaced by 26, a small deformation, inversely proportional to constant K , will follow. If, on the other hand, $\underline{\underline{\delta\sigma}}$ is orthogonal to the initial stress tensor, its application will entail a small strain increment $\underline{\underline{\delta\epsilon}}$, such that the new strain tensor will be exactly the point of Σ where the orthogonal direction is that of the new stress tensor. In this second case, the apparent elastic modulus is thus inversely proportional to the curvature of surface Σ .

In spite of the analogy, presented in paragraph B.7, between the backbone of the force-carrying structure and cost-minimizing directed paths for scalar transport, the statistical properties of those two systems are quite different. In agreement with various results on disordered systems of grains [8, 47] the triangular lattice system was found [9, 15, 17] to possess a standard thermodynamic limit: intensive quantities like the density of the backbone, the strains, the distribution of contact force values have limits in the limit of large system size (except for

marginally supported loads). On the other hand, unlike the force-carrying structure in the mechanical problem we have been studying, the optimal directed path in the corresponding scalar problem is a critical object.

The validity of the ASD –that might at first sight appear as a mere technical aspect– is finally a crucial ingredient of the model granular systems that we are studying here. The next section examines some stability properties that are important as soon as one does not resort to the approximation.

VIII. OUTSIDE THE ASD: QUESTIONS OF STABILITY.

We now enforce, on physically acceptable equilibrium states, another requirement: that they should be *stable*. We limit ourselves to the cases when stability can be discussed in terms of a potential energy. If the equilibrium state is a local minimum of the potential energy, then there exists a region of finite extent in displacement space, around equilibrium positions, within which the system is spontaneously attracted to the equilibrium configuration.

Within the ASD, one can only discuss potential variations that are of first order in displacements. When floppy modes exist ($k > k_0$), they appear as marginally unstable and one cannot tell whether, to higher orders, they actually destabilize the equilibrium configuration. The mechanical response to small perturbations or load increments is strongly dependent on these stability questions.

In general, we will show, with examples (section A), that the answer might depend on quite specific geometrical features of the granular system, and on the contact law. We are only able to give general answers for spheres or discs, as shown in section B. Section C discusses some consequences on the geometry and coordination of granular packings at equilibrium, and on the macroscopic mechanical behaviour.

A. Simple examples.

We consider rigid frictionless particles of various shapes, and discuss the stability of simple configurations, that depends on the ability of contacts to withstand tension, and on the shape of the grains.

1. Bond alignments.

Assume three spheres, or three discs in 2D, to have their centers aligned as on fig. 11, the two extreme ones being submitted to opposite forces in the direction of the line of centers. Let us discuss the problem in 2D. The determination of contact forces is an isostatic problem, and there is, apart from rigid body motions, a trivial

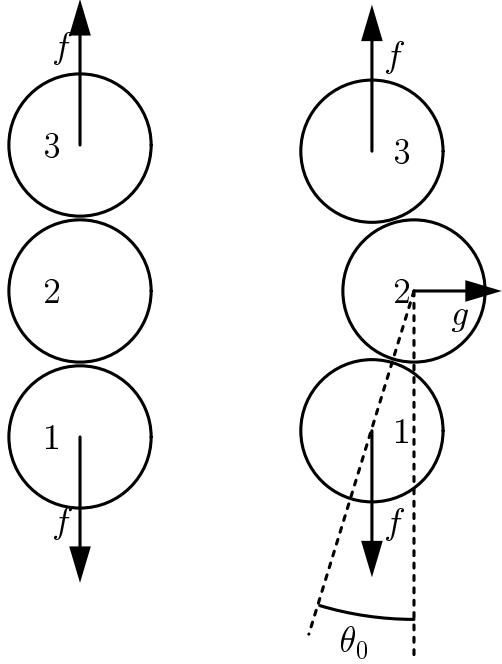


FIG. 11: An alignment of 3 spheres (left), the middle one touching the other 2. Spheres 1 and 3 are submitted to equal and opposite forces along the line of centers. The new equilibrium configuration, upon exerting a lateral force g on the middle sphere, is shown on the right.

mechanism corresponding to free lateral motion of the middle disc 2. This is of course well known to lead to the familiar buckling instability if one pushes the extreme discs towards each other, and to be stable if one pulls on them, provided the contacts can resist tensile forces. In the latter case, assuming one controls the forces parallel to line 1-2 exerted on particles 1 and 3, while their position in the other direction is fixed, the system will respond *elastically* to a small additional force exerted on disc 2, even though the contact law is rigid. After the system reaches its new equilibrium state, the orientation of contacts is such that the new load is orthogonal to the floppy mode. Specifically, if g is the lateral force pulling disc 2 away from the line 1-3, and if f denotes the external force exerted on 1 and 3, the new position of the center of disc 2 is such that, assuming equality of the 3 radii, the angle θ_0 between 1-3 and 1-2 (fig. 11) is given by

$$\theta_0 = \tan^{-1}\left(\frac{g}{2f}\right),$$

while contact forces (tensile, and therefore negative) are

$$f_{12} = f_{23} = -f \cos(\theta_0).$$

The potential energy, as a function of θ (θ parametrizes the free motion that maintains the two contacts), reads

$$W = -2af \cos(\theta) - ag \sin(\theta) = -a\sqrt{4f^2 + g^2} \cos(\theta - \theta_0),$$

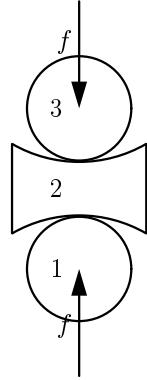


FIG. 12: An alignment like that of fig. 11, the middle sphere being replaced by an object turning concave parts of its surface towards spheres 1 and 3.

and has its minimum for $\theta = \theta_0$.

This elastic behaviour is similar to that of a rigid string under tension, which will deform in response to lateral solicitations.

On carrying out the same calculations in the case of compressive forces, with $f < 0$, one will notice that g and θ_0 , corresponding to the equilibrium position of disc 2, are now of opposite signs. One then has

$$W = a\sqrt{4f^2 + g^2} \cos(\theta - \theta_0),$$

which is *maximized* in the unstable equilibrium position $\theta = \theta_0$.

In section VIIIB, we show that the conclusions reached on this simple example are general: any floppy mode in a system of discs or spheres that admits only compressive contact forces leads to an instability. If, on the contrary, all contact forces are in fact tensile, the system being thus analogous to a network of tight strings, any floppy mode is stable, and an elastic response to small load increments can be observed.

Let us now replace disc 2 by a particle presenting concave surfaces toward discs 1 and 3, as shown on fig. 12. The system is similar to that of fig. 11, the free lateral motion of the middle particle, maintaining the contacts, is a mechanism. It is not difficult to show, however, that the configuration of fig. 12 has, compared to the alignment of discs, *opposite* stability properties: the mechanism is stable for compressive forces, unstable for tensile ones. Thus stability properties are quite sensitive to particle shape.

2. Arches.

Systems submitted to gravity provide other familiar examples of non-rigid equilibrium states. A string of circular, or spherical, particles, each of them tied to two neighbours by a frictionless contact condition that supports tension, behaves as a chain, and will eventually

adopt a stable equilibrium configuration if one fixes its two extremities and let it dangle under its weight. The number of mechanisms in this system is equal to the number of free particles.

The analogous system to the chain, in which contacts transmit compressive forces, is the arch, fig. 13. The general result for spheres entails that all arches made of spheres are unstable. However, one usually builds arches with appropriately shaped stones, *e.g.*, carving them to share common flat lateral surfaces with their neighbours, as on fig. 13. Such an arch is a system that possesses one

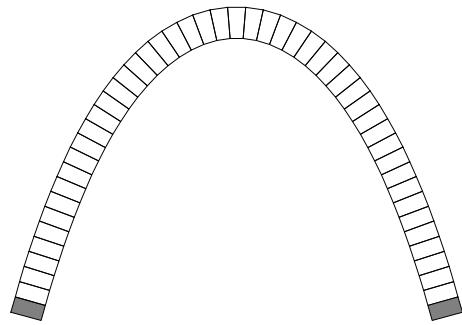


FIG. 13: An arch built with stones sharing flat lateral surfaces.

floppy mode per stone (still assuming no friction), but its geometry might be adequately chosen to support the load. In such a case, any free motion of the stones, that slide on their flat common surfaces, all contacts being maintained, does not change the potential energy. One thus has an example of *marginal stability*. Such an arch is only able to carry the one particular load for which it was specifically designed. (Any amount of friction, however, stabilizes the system).

3. A stable mechanism with strictly convex cohesionless grains.

In view of the previous examples, one might be tempted to infer that mechanisms, when contacts only support compression, can be stable with concave grains (fig. 12), are sometimes marginally stable with flat surfaces (fig. 13), but are always unstable with strictly convex grains (fig. 11). This is however not true, as shown by the simple example of fig. 14. We are not aware of other general answers to this question of stability than the ones that are given for spheres below.

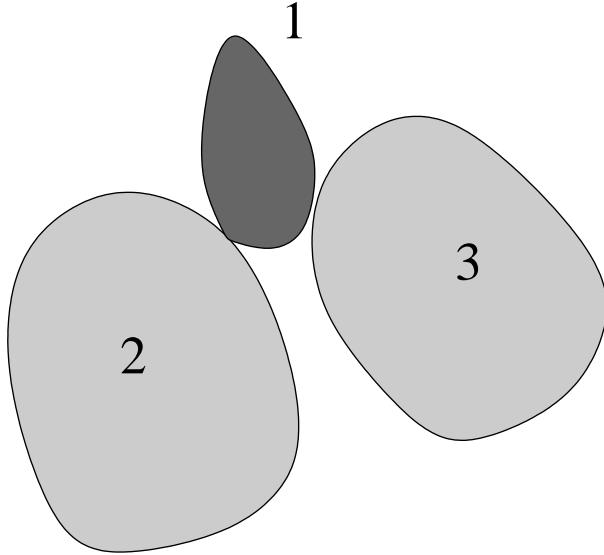


FIG. 14: The upper grain 1 relies on two of its neighbours and is submitted to its weight, oriented downwards. Its rotation is a stable floppy mode.

B. General results for spheres and discs.

1. Tensile contact forces (systems of cables).

In the case when all contacts, at equilibrium, carry a tensile force, then stability is immediately proved once it is realized, as remarked in section VIIA, that minimizing the potential energy is a convex optimization problem (see property 1 stated in section VIIA).

Just like for the simple example of figure 11, floppy modes can exist in stable equilibrium configurations. Then, the system will respond elastically to small load increments that provoke small motions of those floppy modes. Applying such load increments amounts to slightly deform the potential energy landscape on the manifold of configurations that maintain the initially existing contacts. A new minimum is found, close to the previous one.

Systems of rigid cables, *whatever the level of deformation*, should therefore possess exactly the same kind of elasticity, due to preexisting stresses, as assemblies of rigid frictionless particles without cohesion *within the ASD* (whose mechanical response to load increments was discussed in section VII.E).

Those properties were in fact discussed by Alexander [40], in his monograph on the elasticity of various kinds of networks and amorphous systems, in the case when the contact law is *elastic*. Alexander pointed out that stable configurations are not necessarily rigid. He stressed that force-carrying bonds or contacts always have a stabilizing effect when they transmit a traction, and a destabilizing one when they transmit a compression.

Our present study, in this subsection, might be re-

garded as complementary to his, since we deal with *rigid* contacts.

2. Cohesionless grains.

Let us now show that, in the absence of tensile force in the contacts, an equilibrium configuration of rigid, frictionless discs or spheres is necessarily unstable if the backbone is not a rigid structure.

We shall do so by yet another application of the theorem of virtual power, as follows.

We assume a packing of spheres to be in equilibrium under a prescribed load. Spheres are rigid, and the problem is therefore isostatic, $h = 0$. Flat walls can also exist, *e.g.*, as a device to enforce some kind of boundary condition on the packing, but we assume that they cannot rotate. We assume there is at least one mechanism: $k \geq 1$. Consequently, it is possible to move the grains (and the walls) while maintaining the whole list of contacts. (The possibility that a mechanism could exist for the considered equilibrium configuration alone, and disappear as soon as the grains are displaced is to be discarded as non-generic. This would, in particular, due to 16, entail $h \geq 1$). We now study the variation of the potential energy in one such motion, with a ‘time’ t parametrizing the trajectories, and show that it decreases.

Objects do not rotate in this motion (this is an assumption for walls, and rotations of frictionless spheres are ignored anyway). Particle i has a time-dependent velocity $\mathbf{V}_i(t)$, and initially, in the equilibrium configuration from which the motion starts at $t = 0$, touches its neighbour j in a point A_{ij}^0 , where the normal unit vector to its surface, pointing to the center of j , is \mathbf{n}_{ij}^0 , the equilibrium contact force being f_{ij} . Let $A_{ij}(t)$ denote the material point of the surface of grain i that was at A_{ij}^0 initially. Similarly, following the material motion of j , one defines $A_{ji}(t)$, which does not coincide in general with $A_{ij}(t)$. It is possible, at each time t , to apply the theorem of virtual power, thus evaluating $W'(t)$, the time derivative of potential energy W at time t , as follows. The definition of a structure, in part II, was in fact completely arbitrary. Here, let us use this one: at time t , although objects i and j that are in contact effectively touch each other by a different point, define a bond to exist between $A_{ij}(t)$ and $A_{ji}(t)$, oriented by \mathbf{n}_{ij}^0 , which, because objects do not rotate, is still carried by the common normal direction to the surfaces of i and j at these two points. This structure might be used to define virtual, fictitious bond forces, that we choose equal to the initial equilibrium contact forces, *i.e.*, f_{ij} , carried by \mathbf{n}_{ij}^0 in the bond between $A_{ij}(t)$ and $A_{ji}(t)$. These forces are now used in the theorem of virtual work, with the real velocities. This is perfectly valid, because for each t

- the virtual internal forces balance the constant load
- in the bond between i and j , the force exerted on i is still equal to the opposite of the force exerted on

j .

One obtains:

$$W'(t) = \sum_{i < j} f_{ij} \mathbf{n}_{ij}^0 \cdot (\mathbf{V}_j(t) - \mathbf{V}_i(t)),$$

the sum running over all bonds. As $f_{ij} \mathbf{n}_{ij}^0$ does not depend on t , this is easily integrated. Denoting as $\mathbf{U}_{ij}(t)$ the vector of origin $A_{ij}(t)$ and extremity $A_{ji}(t)$, the net variation of potential energy at time t , from the beginning of the motion is

$$W(t) - W(0) = \sum_{i < j} f_{ij} \mathbf{n}_{ij}^0 \cdot \mathbf{U}_{ij}(t). \quad (48)$$

In the motion, $A_{ij}(t)$ and $A_{ji}(t)$ are still extreme points of solids i and j in the respective directions \mathbf{n}_{ij}^0 and $-\mathbf{n}_{ij}^0$. As spheres i and j have stayed in contact, it follows that, as shown on figure 15, the contribution of bond $i-j$ to 48 is strictly negative, unless $A_{ij}(t) = A_{ji}(t)$, in which case it is zero. The same conclusion holds true for a contact

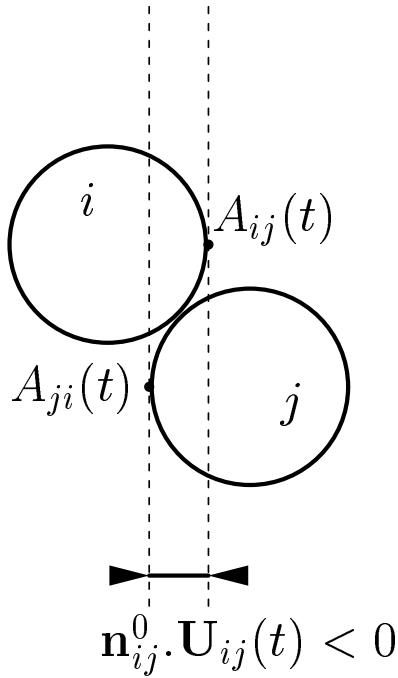


FIG. 15: Sketch of the position, at time t of two spheres in contact.

between a sphere and a flat wall that does not rotate. Consequently, one must have:

$$W(t) - W(0) < 0,$$

unless all intergranular contacts that carry non-vanishing equilibrium forces are maintained, in the motion, via the same material points. This latter condition means that the backbone of the contact structure in the equilibrium configuration moves as a rigid body.

Mechanisms that only affects grains that do not carry any force, without altering the geometry of the backbone will not, of course, change the value of W and lead to instabilities.

Otherwise, the instability is always present. We have shown that *the backbone of the contact structure*, in a stable equilibrium configuration of a packing of rigid, frictionless spheres that do not support tensile forces in the contacts, *is devoid of mechanisms other than rigid-body motions*: $k = k_0$. As we already knew, from part VI, that it cannot possess self-balanced contact forces ($h = 0$), one reaches the conclusion that *it is an isostatic structure*.

C. Consequences. Discussion.

1. Coordination of packings.

The isostaticity of the force-carrying structure in packings of rigid frictionless *spheres* with contact law 21 thus results from a stability analysis. The opposite inequality to the ones established in section VI.D, can, in this case, be stated: one has $N \geq N_f$, and consequently, $N = N_f$, on the backbone of the contact structure. For large systems, the absence of floppy mode implies a *lower bound* on the coordination number:

$$c \geq 2d \quad \text{on the backbone.}$$

This is equal to upper bound 33, hence the equality: $c = 2d$.

However, for frictionless grains with different shapes, or for spheres with cohesion, one cannot expect in general inequality 33 to hold as an equality, even on the sole backbone.

Returning to cohesionless packings of spheres, when each one is submitted to an external force, it has to belong to the force-carrying backbone, and the whole system satisfies $N = N_f$ (or, asymptotically for large sizes, $c = 2d$). This happens in system A, treated without resorting to the ASD. The force-carrying structure that was obtained, SA2, is isostatic and spans the whole system. When external forces are transmitted from the boundary, as in system C, floppy modes can exist, typically as isolated spheres, like discs 10 and 14 on fig. 3, or small sets of spheres, that are not or insufficiently connected to the backbone. If not too widely polydisperse systems of spheres, regions that are totally shielded from force transmission are usually quite small. According to our experience in numerical simulations, if the ratio of the largest to the smallest radius is 2 in a polydisperse assembly of discs, then one very rarely sees more than 3 discs together in such regions. In 2D, ring-like arrangements surrounding discs that carry no force, such as 29–30–31–15–6–5–13–28 and 11–3–9–22–23–24 on fig. 3, cannot easily be made very large: the curvature of the ‘ring’ would then decrease, increasing the risk of inward buckling.

2. Lattice models with and without the ASD.

The triangular lattice model, as defined in section IV.B, of which systems A and B are particular samples, provides vivid examples of the difference between tensile contacts (systems of strings, satisfying 23) and compressive ones (rigid grains obeying 21), once dealt with outside the ASD. Within the ASD, both types of systems share the same properties, and an equilibrium state of one of them can be mapped onto an equilibrium state of the other, as follows. In the reference state, rigid discs do not touch, since $h_{ij}^0 = (a/2)(\delta_i + \delta_j)\alpha > 0$. This can be mapped onto a string network system, in which the ‘contact law’ is 23, on replacing each δ_i by $-\delta_i$ and attributing the length $a(1 + \alpha(\delta_i + \delta_j)/2)$ to the string joining i and j . On reversing the sign of external forces, an exact correspondence is achieved between equilibrium states.

Fig. 16 shows the force-carrying structure, as obtained within the ASD, in a hexagonal sample (for one random choice of δ_i values, drawn according to a uniform distribution) of 1141 discs. This system is submitted to an isotropic pressure, via a imposed homogeneous shrinking of the perimeter.

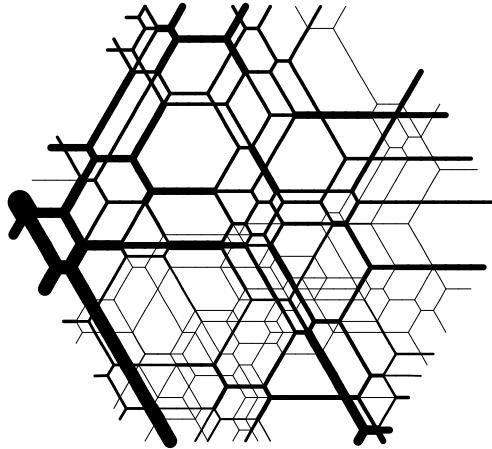


FIG. 16: Triangular lattice model, within the ASD: force-carrying structure S^* in a hexagonal sample submitted to an isotropically compacting load. Line widths are proportional to force intensities. The very same structure is observed in a corresponding system of strings undergoing isotropic tension.

As established in section VII B, such a structure is, within the ASD, only dependent on the random parameters δ_i . The dynamics ruling the motion of the particles from the reference to the equilibrium positions, and the actual value of α are both irrelevant. In the corresponding system of strings submitted to isotropic tension, ex-

actly the same force pattern is obtained at equilibrium. We denote as S^* the backbone of the contact structure, as displayed on fig. 16. Just like in structure SB1, which carries the force in a similar sample of smaller size, many discs do not belong to S^* , which only contains 619 of them, thus possessing 1239 degrees of freedom (counting the one of the ‘wall’). Many floppy modes are present, 381 of them are associated with bond alignments (discs having two contacts in opposite positions), and the remaining 5 are more collective (like the one of fig. 6). Some statistical properties of S structures in the large system limit were studied in [15].

We numerically determined force-carrying structures in the rigid disc system under compression, and in the corresponding system of strings under tension, without the ASD. Those structures, that were obtained with $\alpha = 1/48$ (this value is now relevant), are respectively denoted as SC and ST , and shown on figures 17 and 18. Slight

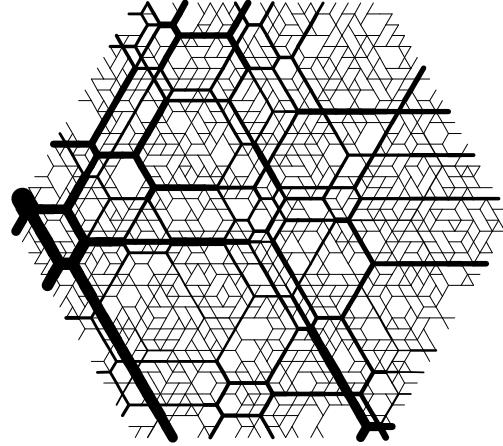


FIG. 17: Structure SC that replaces S^* outside the ASD in the case of contacts resisting compression.

distortions of the regular triangular lattice, although not apparent on the figures, were taken into account in the calculations. From part VII, we know that ST is still determined by the sole system geometry: since forces are the solution to a convex optimization problem, the uniqueness property still holds. This is not the case for SC , and the result now depends on the actual dynamics (the rule that was adopted to move the discs to their final equilibrium positions). The calculation was carried out with the ‘lubricated granular dynamics’ method of refs. [9, 15].

As expected, SC is devoid of mechanisms: it is an isostatic structure, with 1052 discs, 2105 degrees of freedom, and exactly 2105 contacts. Only 89 grains out of the total number 1141 do not belong to SC . Most of them are isolated grains, or pairs of neighbours (slightly larger re-

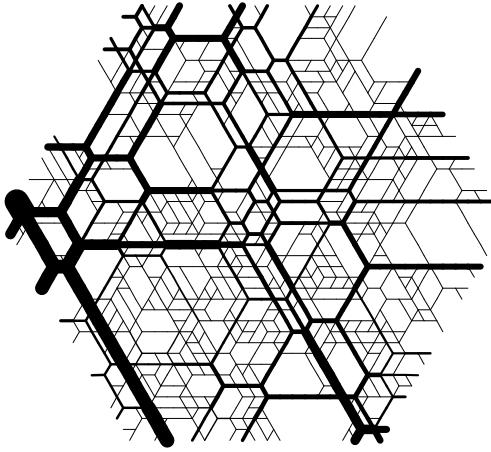


FIG. 18: Structure ST that replaces SC for an analogous system of cables resisting tension.

gions shielded from the forces appear near the perimeter, due to a boundary effect).

On the other hand, ST stays more tenuous, with 840 discs only, and 1401 contacts. Thus 280 floppy modes still live on ST , 232 of which are simple bond alignments and 48 are collective.

In spite of those differences between the density of S^* , SC and ST , it does appear on the figures that the spatial distribution of the forces is very similar, the strongest ‘force chains’ remaining unaltered. The distributions of force values in S^* and SC , in the limit of large systems were evaluated in ref. [15], and shown to coincide, within statistical uncertainties, except for the small forces that appear on SC in the additional contacts created by the buckling instabilities in S^* .

Thus, resorting to the ASD is quite a legitimate procedure, provided α is small enough as to allow to regard the differences between SC or ST on the one hand, and S^* on the other, as refinements that can be neglected.

In the limit $\alpha \rightarrow 0$, any contact force on SC is expected to tend to its value in S^* , although the density of force-carrying contacts is discontinuous.

In the system of strings under tension, on the other hand, mechanisms do not lead to instabilities, and the density of the backbone itself should continuously approach that of S^* as $\alpha \rightarrow 0$.

3. Role of grain shape: are spheres special ?

We have seen that it is necessary to examine, beyond the ASD, questions of stability, to find qualitative differences between intergranular contacts that resist compression and cables that resist tension, and between spheres

and other shapes.

Of course, one expects macroscopic properties of granular assemblies to smoothly depend on grain shape: packings of nearly spherical grains will resemble packings of spheres. Experimentally, it has sometimes been observed that systems of spheres, in a quasi-static experiment, yield particularly noisy responses. It is also empirically known in civil engineering that granulates made of smooth and rotund particles, like river-bed gravel, are especially unstable and prone to large plastic deformations.

Unfortunately, detailed data at the microscopic level on non-spherical grains close to equilibrium are scarce.

Although detailed analyses of such features are lacking, and our study of granulate stability should be extended to the case of spheres with friction, one might speculate that such particular behaviours of rotund objects could be related to the specific property we have established here: whenever some motion is smoothly initiated (*i.e.*, with a very small initial acceleration), while existing force-carrying contacts are maintained, then it will entail some loss of potential energy, and thus accelerate further. Hence probably the jerky aspect of system trajectories in configuration space.

Section IX discusses, precisely, when and how a system jumps from one equilibrium state to another.

IX. MECHANICAL RESPONSE TO LOAD INCREMENTS: TOWARDS MACROSCOPIC BEHAVIOUR.

So far, we have mainly dwelt on mechanical properties of model granular systems. Those can be proved directly. We wish now to discuss possible macroscopic consequences in terms of the constitutive laws that are relied upon in a continuum mechanics description. We thus have to infer some of the properties of granular packings in the limit of large systems. To be quantitative, some statistical knowledge of the geometry of large granular systems is needed, which requires experiments or numerical simulations. Here, as we do not present new experimental or statistical studies, we shall focus on qualitative properties, extrapolating on the characteristics of finite systems we have been presenting so far, and exploiting some recent numerical results, especially those of ref. [17], recalled in paragraph VII.B.8.

Some macroscopic aspects of granular mechanics are recalled in part A. Possible origins of plasticity are discussed in part B, in relation to grain-level characteristics. Part C examines some consequences of the strong isostaticity property of systems of frictionless spheres without cohesion, in which case some response functions to load increments are related to the operator G , defined in section II in relation to equation 12, corresponding to the isostatic structure. Part D exploits the results of ref. [17], deriving the form of the macroscopic equations to be solved when a small load increment is applied.

Finally, these results are compared, in part E, to some other approaches and theories, that were put forward by several authors in the recent literature, both at the microscopic [33, 34, 35] and the continuum [11, 12, 13, 14] level.

A. Macroscopic granular mechanics: known features, conflicting models.

A classical way (see, *e.g.*, in [19]) to study the macroscopic mechanics of granulates is to submit a sample to a triaxial test. Such a device is designed to impose a uniform state of stress throughout the sample. It does not matter, for our discussion, whether this macroscopic stress is imposed via a fluid pressing on a flexible membrane (as in a laboratory apparatus, for the lateral confinement) or via a control of the position of a rigid wall (as in some numerical simulations). We just need to remember that a varying load is imposed, and depends on two parameters p and q , the axial stress (σ_{yy} on the figure) being equal to $p + q$ and the lateral one (σ_{xx} , to p). A typical experiment consists in gradually increasing q at constant p . One may then observe the resulting strains. The classical elasto-plastic constitutive laws that are ap-

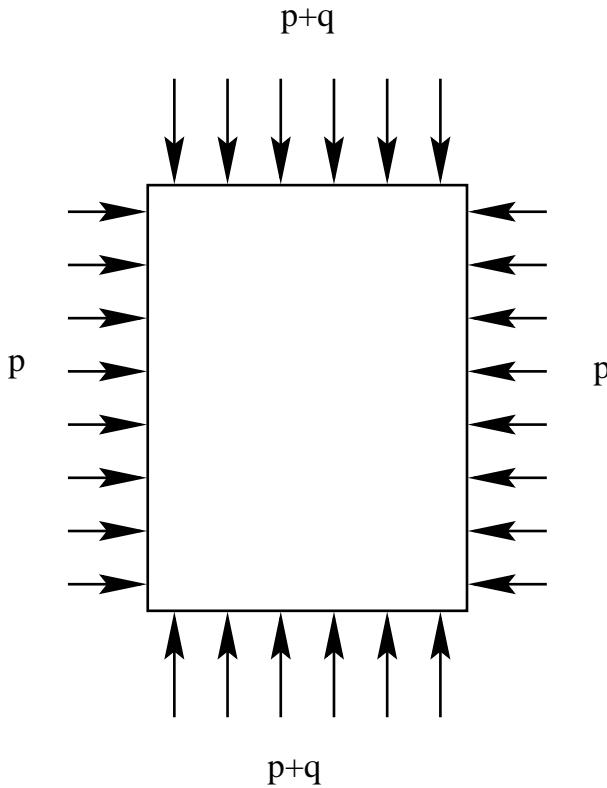


FIG. 19: The triaxial experiment.

plied to granular materials are incremental, which means that they do not relate stresses and strains directly, but predict the increment of strain resulting from an increment of stress, given the current state of the system (the

definition of which might require other, ‘internal’ variables). Cycling solicitations of small amplitude usually yield, in the stress-strain plane, loops with some amount of hysteresis. The surface area of such a loop as OABO on fig. 20 is the plastically dissipated energy associated to deviatoric stresses (to which the work due to volume changes has to be added to get the total plastic work).

In marked contrast with classical soil mechanics approaches, some authors recently proposed a new type of macroscopic mechanical description for the statics of granular packings [11, 12, 13, 14]. According to them, resorting to strain variables should be avoided and one should look for direct relationships between the components of the stress tensor, so that it is possible to determine the whole stress field in a granular sample by solving hyperbolic second-order partial differential equations. Those, like wave equations, possess characteristics, preferred directions along which they reduce to simpler, first order forms. To solve the problem, one may integrate along the characteristics that emerge from every point where some external force is applied. Consequently, in a packing in which the forces exerted on the top boundary (wall or set of particles) are known, a perturbation (external force increment), will *propagate* downwards, but will not be felt above the point where it is applied. The exact relation between stresses to be used should then depend on the actual process by which the sample was made. If the current stress level is changed, by, say, a manipulation of the boundary conditions, like in the triaxial test, then the granular system rearranges until the new constitutive relation, corresponding to its new state, agrees with the new externally imposed stress values. Those theories, in their current state of development, do not predict the extent to which the system has to rearrange, or, in other words, the magnitude of the ensuing strain increment. It has been recently proposed [35] that isostaticity could justify such theories for frictionless assemblies of grains. These suggestions are discussed in section IX.E below.

We now turn to a discussion of some possible microscopic origins of plastic dissipation.

B. Origins of plastic dissipation.

When a given supported external load places the system in a uniquely determined equilibrium state, one has to expect a mechanical behaviour devoid of plastic dissipation. Hysteresis loops like those of fig. 20 cannot occur. Plasticity is related to the lack of uniqueness of equilibrium states. At the level of continuum mechanics, it is sometimes termed ‘internal friction’, since the material behaves as if different layers of matter slided, with friction, on one another within the bulk of the sample. We have thus identified two microscopic origins of *internal friction in systems of frictionless grains*.

1. bounded tensile forces in the contacts (as in section VI.C)

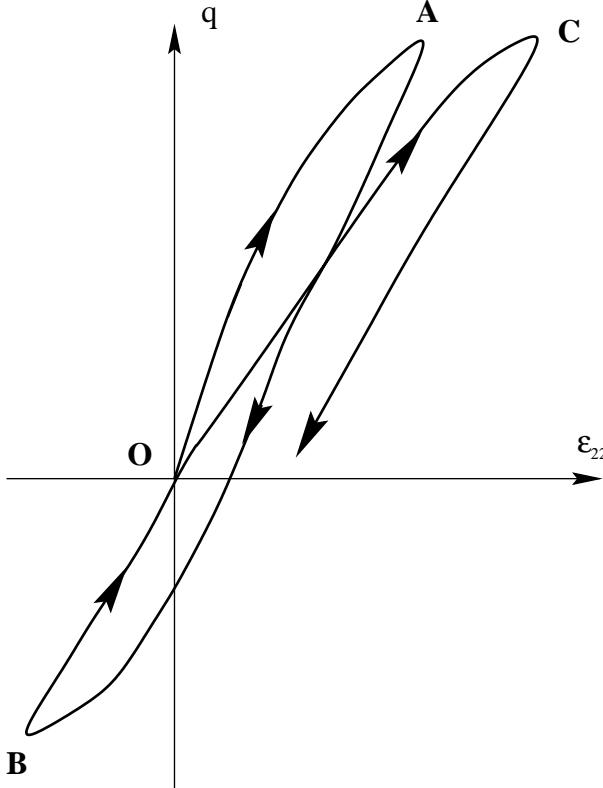


FIG. 20: Schematic aspect of response to cyclic variations in q in the ϵ_{22} - q plane.

2. rearrangements of finite extent (*i.e.*, the ASD is no longer valid) between equilibrium position of assemblies of spherical grains.

Let us illustrate these different behaviours on the simple example of fig. 10 (section VI.C).

Starting from an equilibrium configuration in which the external force on disc 1, in contact with 2 and 3, is vertical, let us gradually increase its horizontal component F_x . We first discuss the problem within the ASD. It is then a particular example of \mathcal{P}_1 discussed in section VII, a linear optimization problem with two unknowns (the coordinates of disc 1). In fact, the simplex within which potential energy W has to be minimized is exactly the one that was shown on fig. 9. Points A and B on that figure are respectively the equilibrium positions of the center of disc 1 when it is in contact with 2 and 3, and with 3 and 4. Changes from one position to the other happen when the direction of \mathbf{F} is orthogonal to that of segment AB. One may monitor the abscissa of the mobile disc, x , which, as presented on fig. 21, is related to loading parameter $Q = \frac{F_x}{F_y}$ via a step-like function.

In analogy with this problem of rigid grains, one may build a system of rigid cables (resisting tension, but not compression), which, if treated within the ASD, yields exactly the same simplex of accessible configurations, the same optimization problem (\mathcal{P}_1) as that of fig. 9. This system of cables is shown on fig. 22. Node 1 is now tied

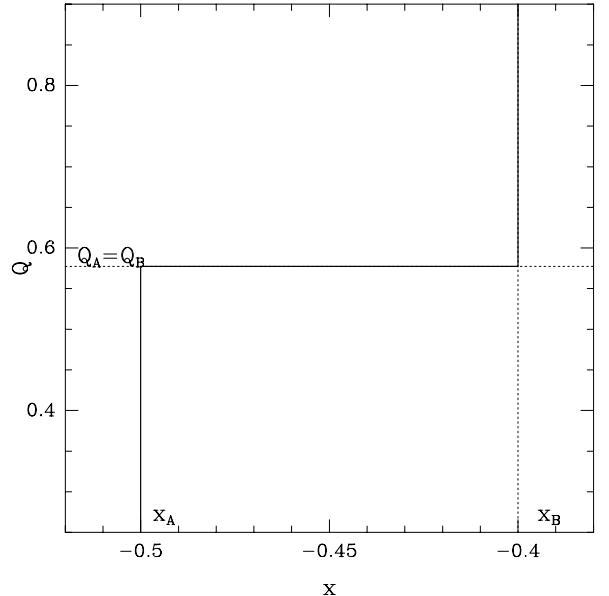


FIG. 21: Loading parameter $Q = \frac{F_x}{F_y}$ versus coordinate x of the mobile disc of the system of fig. 10.

to 2, 3, and 4, by cables that are slightly longer than the common distance between 2 and 3, and between 3 and 4.

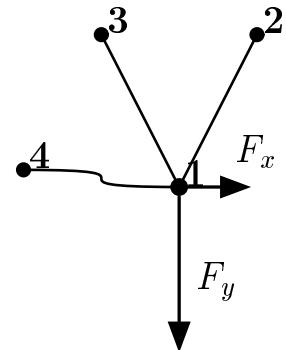


FIG. 22: System of cables, equivalent, within the ASD, to the system of discs of fig. 10, with the same values of external forces. Here, the cables joining 1 to 2 and 3 are taut, while the one joining 1 to 4 is not.

Outside the ASD, the potential minimization problem for the system of cables is no longer a linear optimization problem, but, according to the general properties discussed in section VIII, is still a convex problem. In the plane of the coordinates of node 1, the simplex of fig. 9 changes into a domain limited by curved faces, as shown on fig. 23. The curvature of the faces being oriented inwards, this domain of accessible configuration is convex. When the orientation of force \mathbf{F} is such that, on

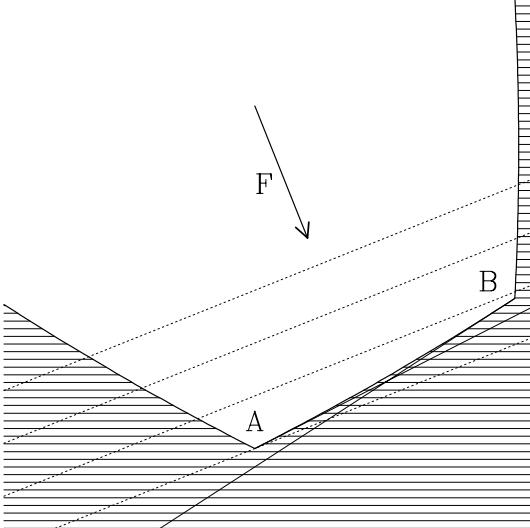


FIG. 23: Minimization problem in the plane of coordinates of node 1, for the system of figure 22 without the ASD. The accessible part of configuration space (outside the hatched zone) is convex. Its boundary has sharp corners (*A* and *B*), but, unlike on fig. 9, corresponding to the same problem within the ASD, displays curvature in between. Tangents to that curve at *A* and *B* are drawn.

fig. 23, the direction of constant potential energy lines lies between those of tangents to the accessible domain in *A* and *B*, the equilibrium position is a point on arc *AB*, and only one cable is taut, the one joining 1 to 3. In this case, the motion along arc *AB* is a mechanism, but stability is maintained, just like in the example of fig. 11. There is still a one-to-one correspondence between $Q = \frac{F_x}{F_y}$ and x , as shown on fig. 24. As the difference between cable lengths and distances 2-3 and 3-4 decreases, displacements get smaller and smaller. The difference $Q_B - Q_A$ tends to zero, the curvature of the accessible region boundary on fig. 23 vanishes, and the curve of fig. 24 approaches the ASD case, fig. 21. Over a finite interval between Q_A and Q_B , the force-displacement relationship is a smooth function, unlike the stepwise dependency shown on fig. 21 (corresponding to the limit of very small motions).

Let us now deal with the system of fig. 10 (with rigid, impenetrable discs and frictionless contacts that do not resist tension) *outside the ASD*. The accessible domain in the coordinate plane is, as opposed to the previous cases, no longer convex, as shown on fig. 25. The upper limit Q_A of the Q interval for which position *A* is stable is now larger than the lower limit Q_B of the Q interval for which position *B* is stable. Because of this *bistability* for $Q_B \leq Q \leq Q_A$, the Q versus x relation now exhibits hysteresis, as shown on fig. 26.

As shown in section VI.C, contact law 25, that allows for some bounded tensile forces in the contacts, is such

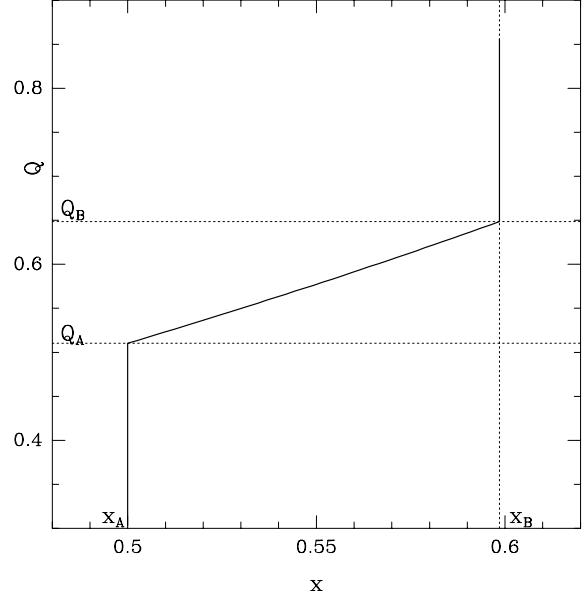


FIG. 24: Force ratio Q versus coordinate x of node 1 for the system of fig. 22, without the ASD.

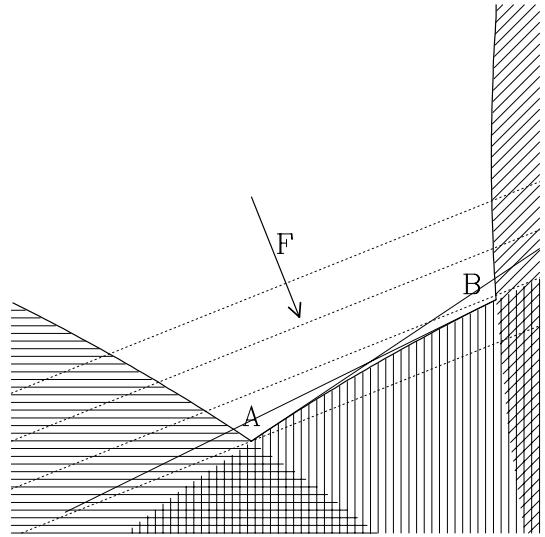


FIG. 25: Same as figs. 9 and 23, in the case of the system of fig. 10, without the ASD. The straight lines are the tangents to the boundary curve at points *A* and *B*.

that both equilibrium positions *A* and *B* will be simultaneously possible for some values of Q , in the system of fig. 10. Q then varies with x exactly as shown on fig. 26,

$$\text{with } Q_A = \frac{1}{\sqrt{3}} + \frac{f_0}{F_y} \text{ and } Q_B = \frac{1}{\sqrt{3}} - \frac{f_0}{F_y}.$$

One may note, however, that the plasticity due to cohesion of finite strength differs from the one due to geometric rearrangements in the two following respects.

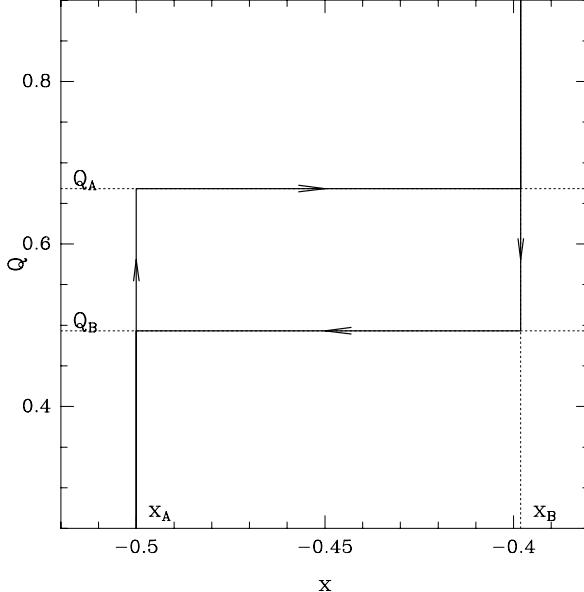


FIG. 26: Same as figs. 21 and 24, in the case of the system of fig. 10 outside the ASD. The force-displacement relation is now history-dependent, as shown by the arrows.

- With contact law 25, plasticity does not disappear in the limit of small motions (when the ASD becomes valid).
- It is sensitive to the *magnitude* of external forces, not only on their *direction*. The figure analogous to 26, in the $(Q = \frac{F_x}{F_y}, x)$ plane, now depends on the value of F_y . When F_y is very much larger than f_0 , the cohesive strength of contacts might be neglected, and vanishes as a source of plastic dissipation.

It might be expected, on going, from the elementary example dealt with in this section, to larger and larger systems, that curves like fig. 26, forces (like F) averaging to stresses and displacements (like x) to strains, will gradually look like fig. 20. In larger systems, the curve of fig. 26 will look like a staircase. Presumably, as the system size increases, the number of the steps, and their amplitude, if expressed in terms of intensive quantities, will tend to zero. Then the smoothness of the curves sketched on fig. 20 *might* be recovered in the thermodynamic limit. Whether it actually *will* is of course not obvious a-priori, a careful statistical analysis [49] is required. In the case of systems treated within the ASD, each step of the resulting staircase will be retraced back and forth, without any irreversibility. Such models can be expected to share the properties of the lattice system of ref. [17] and paragraph VII.B.8, in which the staircase does indeed approach a smooth stress-strain curve in the thermodynamic limit. (But this curve is unique, one cannot obtain fig. 20 in such a case).

The difference between plasticity of cohesive and non-cohesive grains that was pointed out above is reminiscent of the difference in the behaviour, under growing hydrostatic pressure, of sands and clays [19]. As the magnitude of the load increases (but its direction is fixed), the level of plastic deformation in the cohesive material (clay) is much higher than in the non-cohesive one (sand).

It is also interesting to note that some theories of friction between solid surfaces [48] are, just like the mechanisms for *internal* friction that we invoke here, based on the history-dependent selection of one among several possible stable equilibrium configurations.

C. Consequences of isostaticity.

We focus here on systems of frictionless, cohesionless and rigid spheres (the contact law being 21) in equilibrium under a given load, for which it was shown, in two steps (sections VI and VIII), that the force-carrying backbone is an isostatic structure. We discuss some specific consequences of this property. In the simple example treated in subsection B just above, both equilibrium configurations A and B correspond to isostatic contact structures, and it is easy to predict for which value of the loading parameters the system will change from one to the other. Exploiting the isostaticity property, we will show here that such a prediction can, to some extent, be done in an arbitrary system.

In this subsection, we only consider the backbone, ignoring the rest of the system. We suppose that grains have been renumbered, so that index μ , with $1 \leq \mu \leq N_f$ only label the degrees of freedom of objects that belong to the backbone. We shall also adopt the convention that the whole backbone does not move as a rigid body (thus excluding the k_0 corresponding degrees of freedom from the list). Likewise, $1 \leq l \leq N$ here only labels the force-carrying contacts ($N = N_f$).

1. Response to perturbations, without rearrangement.

Isostaticity of the whole structure means that matrix G , and its transpose G^T are square and have an inverse. Not only are equilibrium forces, given the load, uniquely determined, but it is also possible to predict how small external force increments (on the backbone) will be distributed in the existing contacts. Changing the load from $(F_\mu^{ext})_{1 \leq \mu \leq N_f}$ to $(F_\mu^{ext} + \delta F_\mu^{ext})_{1 \leq \mu \leq N_f}$ will result, in contact l , in force increment δf_l , given by (summation over repeated indices implied)

$$\delta f_l = (G^T)^{-1}_{l\mu} \delta F_\mu^{ext} = G^{-1}_{\mu l} \delta F_\mu^{ext}. \quad (49)$$

The backbone being rigid, this change in forces does not entail any displacement: $u_\mu = 0$ for each μ . This correctly describes the mechanical response of the granular assemblage as long as all contacts forces remain positive.

This should be the case, in a finite system, for sufficiently small perturbations of the initial load.

2. Dual response of velocities to bond length variations.

Parallel to the one-to-one correspondence between contact forces and external loads expressed by eqn. 49, is the inversible linear mapping between velocities and relative normal velocities in the contacts. There is no compatibility condition in the absence of hyperstaticity, and one may impose arbitrary values to relative normal velocities $(\delta V_l)_{1 \leq l \leq N}$ for the whole list of contacts. The resulting velocities of the spheres are then (summation over l implied) :

$$V_\mu = G_{\mu l}^{-1} \delta V_l. \quad (50)$$

On comparing to 49, it appears that the same matrix element $G_{\mu l}^{-1}$ is both equal to the force increment in contact l created when a unit external force is exerted on the coordinate μ on the one hand, and to the velocity coordinate μ when δv is equal to one in contact l and to zero in all other contacts, on the other hand. Such a symmetry in response functions was remarked by Moukarzel [34], who derived it by different means.

3. Response to perturbations: structural rearrangements.

The particular form of mechanical response expressed by eqn. 49, in which no motion occurs and the load increment is supported by the initially existing contacts, ceases to be relevant as soon as negative contact forces appear. In the case of a two-parameter loading mode, such as the biaxial experiment at constant p , in which q is gradually increased from its initial value $q = 0$, one may write in each contact l

$$f_l = \beta_l p + \gamma_l q,$$

where β_l and γ_l are, due to isostaticity, geometrically defined coefficients. In general one finds that some of the γ_l are negative. Let us denote as L^- the set of such contacts. The load will no longer be supported as soon as q reaches the value

$$q_{max} = \min_{l \in L^-} \frac{-\beta_l}{\gamma_l} p. \quad (51)$$

For larger q 's, the theorem of virtual power shows that it is possible to decrease the potential energy upon opening the contact l_0 for which the minimum in the right-hand-side of 51 is reached, all other contacts remaining closed. The system will then rearrange, until a new set of contacts is created, such that the new load (p, q) is supported with positive contact forces. If one uses the ASD to describe this motion, then, within this approximation, the new list of contacts, as shown in section VI,

is entirely determined by the sole system geometry, as the solution to a simplex problem. Outside the ASD, the new equilibrium state, after the system rearranges, might depend on specific dynamical laws. In general, the range of validity of the ASD and the influence of the dynamics are to be tested, in experiments or, perhaps more easily, in numerical simulations. However, we have just shown, in fact, that *the direction of velocities at the beginning of the rearrangement* is determined by purely geometrical conditions, at least if l_0 is unique: to find those directions, just impose $\delta V_{l_0} = -1$ (thus opening contact l_0), and $\delta V_l = 0$ for any $l \neq l_0$, from which all velocity components are deduced as $v_\mu = -G_{\mu l_0}^{-1}$, from equation 50.

Simulations of disordered systems of discs [50] suggest that l_0 is generically unique, except in situations when the opening contacts involve a cluster of $d+1$ -coordinated spheres in d dimensions. Examples of such clusters are sets of discs 8, 19 and 2, or 6 and 15, or 12 alone on figure 3. It is easily realized that once one contact force involving *e.g.*, disc 8 is known, then all contact forces involving discs 8, 19, or 2 are also known, and proportional to the first one. Thus, they all vanish simultaneously. This means that all matrix columns $(G_{\mu l}^{-1})_{1 \leq \mu \leq N_f}$ are proportional to one another for all indices l that label contacts of d -spheres belonging to the same $d+1$ -coordinated cluster. Returning to the determination of the motion when the load ceases to be supported by the initial list of contacts, it follows that even though, in such a case, several contacts, involving the same cluster of $d+1$ -coordinated spheres, may simultaneously open, the uniqueness of the initial velocities, up to a common amplitude factor, is preserved for all spheres that do not belong to the said cluster.

4. Fragility.

When a rearrangement occurs after a load increment, the mechanical response of the granular assembly, unlike the one expressed by equation 49, involves both force changes *and* displacements. It depends on the possibility of closing contacts that are not present in the initial equilibrium configuration. This geometric information is not contained in matrix G , which only depends on the network of initially existing contacts. One could thus study a second type of response to perturbations, that involves displacements. To see which of the two kinds of response is more relevant for the macroscopic mechanical behaviour, one has to impose perturbations that possess some macroscopic meaning, such as changes of q in a biaxial experiment. Then, assuming, to fix notations, q is increased from zero, two cases need be considered. Either the thermodynamic limit of q_{max} , as defined in 51, is positive, or it is equal to zero. In the first case, there exists a finite interval of stress for which no motion occurs in the continuum limit, and the mechanical response discussed in the preceding paragraphs in terms of the sole matrix G is macroscopically relevant. In the second case the

granular material might be appropriately termed *fragile*, since, in the thermodynamic limit, arbitrarily small macroscopic perturbations provoke rearrangements of the contact structure. Then, any macroscopic mechanical experiment involves displacements, the sole knowledge of one network of contacts that corresponds to a given value of the loading parameters is not sufficient. The response expressed by the sole matrix G is not the macroscopically relevant one.

Our simulations of frictionless rigid discs [17, 49, 50] show that such systems are indeed fragile in this sense.[61].

5. An algorithm to compute a sequence of equilibrium configurations.

This suggests the following procedure to determine the sequence of equilibrium states reached by an assembly of rigid, frictionless, cohesionless spheres under varying load (p,q) , without resorting to *any* dynamical parameter (without introducing any inertia, or mechanism of dissipation).

- 1) Starting from an equilibrium configuration, increase loading parameter q until contact force f_{l_0} vanishes.
- 2) Move grains in the direction determined by the opening of contact l_0 , the others remaining closed. Keep the same prescription for the grain trajectories as for the initial velocities, taking into account the rotation of vectors \mathbf{n}_{ij} , until some new contact l_1 is created, such that the new contact list, replacing l_0 (now open) by l_1 , defines an isostatic structure.
- 3) If, in the new contact structure, the contact forces that balance the load are all positive, a new equilibrium state, corresponding to the new load, has been reached: one may go back to step 1) and further increase q . Otherwise, some contact forces are negative. Pick up the one with the highest tensile force, call it l_0 and go back to step 2), with the new contact list.

This algorithm has been implemented by G. Combe and the present author [50]. We propose to name it the ‘geometric quasi-static method’ (GQSM). It does involve arbitrary ingredients: there is no reason to forbid other openings of contacts once interstice h_{l_0} has reached a finite positive value. Its great advantage is the possibility to compute trajectories from the sole knowledge of the system geometry.

The system evolution, under a varying load, appears as a sequence of equilibrium states that are separated by ‘jumps’ or rearrangements, in which the list of active contacts is altered. In a phase of equilibrium, the forces are carried by a minimum list of contacts. In a phase

of motion, normal relative velocities, among the whole bond list, are localized on *one* bond (several if a structure – a list of bonds– larger than the contact structure, is considered). Both *maximum localization phenomena* are related to geometric constraints.

The predictions of the GQSM algorithm were compared with those of other methods that resort to dynamical models (and, as argued in the introduction, also involve arbitrary, non-physical features). The results will be presented elsewhere. As mentioned above, mechanical properties, at the level of individual trajectories in configuration space, cannot be expected, outside the ASD, to be uniquely determined. However, in view of the important role of the geometry, which determines exactly the value of the loading parameters for which system should rearrange and the direction of the initial velocity vector, it can be hoped that the statistical properties of such trajectories that are relevant for the macroscopic laws will present little dependence on dynamical features of the system (such as masses or dissipative shock laws).

6. Rearrangements within the ASD.

Within the approximation, as the equilibrium state corresponding to a given load is unique, there is no need to resort to an incremental approach. If one however does so, then the whole rearrangement event is geometrically determined. It can be computed with the GQSM as presented above. Then, it will be observed, on performing step 3) of the algorithm, that the new contact structure, as soon as a new contact is created, supports the load with only positive contact forces. Thus, unlike in the general case [50], no cascade of successive rearrangements occurs in step 3). Rearrangements are simpler events in which one element of the contact structure is replaced by another.

Let us prove this statement.

Let S_0 denote the old list of contacts, and S_1 the new one. Both structures are isostatic, and for any given load one can find unique values of both sets of bond forces $(f_l)_{l \in S_0}$ and $(f_l)_{l \in S_1}$ that ensure equilibrium. In the following members of these two sets, in order to distinguish them, are written down with a superscript: $f_l^{(0)}$ and $f_l^{(1)}$ respectively denote the force carried by bond l , as computed with structure S_0 and with S_1 .

Recalling also the notations of the preceding paragraph, S_1 is equal to S_0 , deprived of contact l_0 , to which contact l_1 is added. When the value q_{max} of the loading parameter is reached, $f_{l_0}^{(0)}$ has decreased to zero. This means that, exceptionally, the smaller structure $S_0 \setminus \{l_0\} = S_1 \setminus \{l_1\}$ can support the load, and one has $f_{l_1}^{(1)} = f_{l_1}^{(0)}$, while $f_l^{(1)} = f_l^{(0)}$ for each $l \in S_0 \setminus \{l_0\}$. As we assume, for simplicity, that contact forces reach zero separately, there exists a finite range of positive increments δq such that one has $f_{l_0}^{(0)} < 0$, while $f_l^{(0)} > 0$ for $l \in S_0 \setminus \{l_0\}$, for $q = q_{max} + \delta q$. Likewise, reducing the

δq interval if needed, we require the condition $f_l^{(1)} > 0$ for $l \in S_1 \setminus \{l_1\}$.

We now pick up one such value of q , and evaluate the variation δW of the potential energy (that corresponds to this value of q) in the rearrangement.

On the one hand, one may obtain δW on applying the theorem of virtual work to structure S_0 . As contact l_0 has opened, the corresponding relative normal displacement is negative: $\delta u_{l_0} < 0$, while $\delta u_l = 0$ for each $l \neq l_0$. Therefore, because $f_{l_0}^{(0)} < 0$, one has

$$\delta W = -f_{l_0}^{(0)} \delta u_{l_0} < 0.$$

On the other hand, one may obtain δW on applying the theorem of virtual work to structure S_1 . As contact l_1 has closed, the corresponding relative normal displacement is positive: $\delta u_{l_1} < 0$, while $\delta u_l = 0$ for each $l \neq l_1$. Therefore, because $\delta W = -f_{l_1}^{(1)} \delta u_{l_1} < 0$, one has

$$f_{l_1}^{(1)} > 0.$$

Thus, the new contact structure supports the load with positive contact forces as soon as $q > q_{max}$, and a new stable equilibrium state has been reached.

In the general case, we stressed the difference between the mechanical response of the granular system without rearrangement, which can be deduced from the geometry of the contact structure, *via* matrix G , and the mechanical response involving some rearrangement, the determination of which requires some additional prescription (such as that of the GQSM) to move the particles.

This difference is much less important within the ASD: as the matrices G pertaining to either structure do not change in the motion, all displacement coordinates will simply be found as follows:

$$u_\mu = h_{l_1} G_{\mu l_1}^{-1}, \quad (52)$$

where h_{l_1} denotes the initial opening of contact l_1 and the matrix G is that of structure S_1 .

Equations 50 and 52 only differ by a scale factor, interstice h_{l_1} . There is nothing especially singular in the distribution of open interstices in dense granular systems at equilibrium. So, it can be expected that macroscopic averages corresponding to both response functions, 50 and 52, are proportional to one another. Moreover, the response without rearrangement, expressed by 50, is the same with and without the ASD.

In the following subsection, we derive explicitly the form of the macroscopic response function to small increments in applied external forces, in the case of the triangular lattice model. These are large scale averages of (combinations of) microscopic responses expressed by eqn. 52.

We shall therefore speculate that the results to be derived below, for the form of such macroscopic Green's functions, are also valid for the average of response functions without rearrangements in general.

D. Macroscopic response of the triangular lattice model.

In the model system studied in ref. [17], the results of which are recalled in paragraph VII.B.8, it is possible to find the form of macroscopic equations to be solved when a small density of external forces $\delta \mathbf{f}^{ext}$ is superimposed over an initial equilibrium state.

To do so, one just needs to translate the properties stated in paragraph VII.B.8 in incremental form.

First, let us impose, without loss of generality, a few conditions on function f defined in 45. It is convenient to choose a symmetric function of $\epsilon_{\alpha\beta}$ and $\epsilon_{\beta\alpha}$, the derivation in 46 being taken regarding both strain components as independent variables.

Then, defining, in $\underline{\epsilon}$ space, a norm $\|\underline{\epsilon}\|$ by

$$\|\underline{\epsilon}\|^2 = \underline{\epsilon} : \underline{\epsilon} = \epsilon_{11}^2 + 2\epsilon_{12}^2 + \epsilon_{22}^2,$$

one may enforce (replacing f by $f/\|\nabla f\|$) the condition:

$$\|\nabla f\| = 1, \quad (53)$$

everywhere on Σ .

One starts from an equilibrium state in which the stress field, $\underline{\sigma}$, is assumed to stay strictly inside the supported range, defined by inequalities 42, everywhere in the system. This initial state is also characterized by a displacement field \mathbf{u}_0 and a strain tensor field $\underline{\epsilon}$ (everywhere on Σ , and abiding by 46), the origin being defined by the reference state (the undisturbed regular lattice of spacing a). One then looks for the stress increment field $\delta\underline{\sigma}$, displacement increment field \mathbf{u} and strain increment field $\delta\underline{\epsilon}$ that result from the application of $\delta \mathbf{f}^{ext}$. The problem is dealt with to first order in any of these quantities, that are linear in $\delta \mathbf{f}^{ext}$, assumed small.

Let us define

$$A_{\alpha\beta\gamma\delta} = \frac{\partial^2 f}{\partial \epsilon_{\alpha\beta} \partial \epsilon_{\gamma\delta}},$$

a fourth-order tensor that depends on $\underline{\epsilon}$. One has, upon differentiating the macroscopic law

$$\sigma_{\alpha\beta} = \lambda \frac{\partial f}{\partial \epsilon_{\alpha\beta}},$$

the decomposition of stress increments as

$$\delta\sigma_{\alpha\beta} = \delta\sigma_{\alpha\beta}^{(1)} + \delta\sigma_{\alpha\beta}^{(2)},$$

with (summation over repeated indices)

$$\delta\sigma_{\alpha\beta}^{(1)} = \lambda A_{\alpha\beta\gamma\delta} \delta\epsilon_{\gamma\delta},$$

and $\delta\sigma_{\alpha\beta}^{(2)} = \frac{\delta\lambda}{\lambda} \sigma_{\alpha\beta}$.

Condition 53, yields, by derivation,

$$A_{\alpha\beta\gamma\delta} \frac{\partial f}{\partial \epsilon_{\alpha\beta}} = 0,$$

whence the orthogonality between σ and $\delta\sigma^{(1)}$. Since $\underline{\epsilon}$ must remain on Σ , $\delta\epsilon$ is also orthogonal to σ .

In view of the symmetry of the stress tensor and of the conditions imposed on function f , tensor A satisfies the following symmetries:

$$A_{\alpha\beta\gamma\delta} = A_{\beta\alpha\gamma\delta} = A_{\alpha\beta\delta\gamma}.$$

Because it is a second-order derivative, one also has:

$$A_{\alpha\beta\gamma\delta} = A_{\gamma\delta\alpha\beta}.$$

Tensor A is thus endowed with the same symmetry properties as a tensor of elastic constants (or of viscosity coefficients).

We have seen that it might be viewed as a linear operator within the space of symmetric second-order tensors that are orthogonal to $\underline{\sigma}$, or, in other words, within the tangent plane to surface Σ in strain space. Because of the strict convexity of \mathcal{D} , this operator is *positive definite* (this is easily realized, as the curvature of Σ is turned inwards).

Transforming the equilibrium equation into one for the unknowns \mathbf{u} and $\delta\lambda$, using 43, one obtains (∂_α denoting a derivative with respect to coordinate α)

$$\partial_\beta [\lambda A_{\alpha\beta\gamma\delta} \partial_\delta u_\gamma] - \partial_\beta \left(\frac{\delta\lambda}{\lambda} \sigma_{\alpha\beta} \right) + \delta f_\alpha^{ext} = 0, \quad (54)$$

while the displacement field should satisfy

$$\sigma_{\alpha\beta} \partial_\beta u_\alpha = 0. \quad (55)$$

Equations 54-55, supplemented by suitable boundary conditions, define, because of the positive-definiteness of operator A , an *elliptic boundary value problem*. The solution is unique provided 2 conditions (in 2D) involving \mathbf{u} and/or its normal derivatives are specified everywhere on the system boundary.

We now turn to the situation when the initial stress field is a uniform hydrostatic pressure:

$$\sigma_{\alpha\beta} = P_0 \delta_{\alpha\beta},$$

with a position-independent pressure P_0 . In view of condition 53 on f , it should be noted that λ coincides with $P_0\sqrt{2}$ in this case. The corresponding tangent space to Σ is the space of traceless tensors.

In general, tensor A reflects the common symmetries of the material (the triangular lattice) and the stress tensor. In this particular case, it will possess all the symmetries of the regular triangular lattice. The tensor of elastic constants, in that case [51], has the same symmetries as in an isotropic medium. Because it operates within the space of traceless tensors, tensor A reduces to a scalar K : one has, for any traceless strain increment,

$$A_{\alpha\beta\gamma\delta} \delta\epsilon_{\gamma\delta} = K \delta\epsilon_{\alpha\beta}.$$

54 has become

$$K P_0 \sqrt{2} \nabla^2 \mathbf{u} - \nabla(\delta P) + \delta \mathbf{f}^{ext} = 0,$$

while 55 now states that the displacement field should be divergenceless:

$$\nabla \cdot \mathbf{u} = 0.$$

One recognizes *the Stokes problem for viscous incompressible flow*, in which the displacement replaces the velocity field, the product $K P_0 \sqrt{2}$ plays the role of the shear viscosity, and δP is a pressure field to be determined on solving the full boundary value problem.

Green's functions for the Stokes problem can be found, e.g., in [52]. In an infinite 2D medium, the velocity field varies logarithmically with the distance to the point where a concentrated force is applied.

E. Discussion.

From the results just above, it can be concluded that the form of the macroscopic equations ruling the displacement field created by a small perturbation to a pre-stressed granular sample in equilibrium should be elliptic, provided the microscopic rearrangements are dealt with within the ASD.

From the discussion at the end of paragraph IX.C.6, we expect that operator G^{-1} , in the general case, also averages macroscopically as the Green function of an elliptic second-order partial-differential operator. One may obtain a suitable macroscopic average on taking, e.g., the mean of all matrix elements $G_{\mu l}^{-1}$ for which the vector pointing from bond l to the center of the grain which coordinate μ belongs to is in some prescribed small neighbourhood of a given vector.

G^{-1} rules the response without rearrangement. The general –and, in view of the fragility property, most relevant– case of mechanical response involving rearrangements outside the ASD appears to involve more geometric information than the one contained in matrix G : it could be observed [50] that step 3) of the GQSM algorithm introduced in paragraph IX.C.5 could involve a long sequence of elementary rearrangements replacing one contact by another. Unlike the distribution of open gaps between adjacent particles, that of the magnitude of such complex rearrangements can be quite wide and might significantly affect the macroscopic response in terms of displacements. This will be studied in a forthcoming publication. In the case of a disordered granular assembly, no small parameter, like the level of polydispersity of discs in the triangular lattice model, is available to control the validity of the ASD. As found in section VIII, stable equilibrium states of frictionless discs or spheres are especially scarce in configuration space, as full rigidity is required. Outside the ASD, impenetrability constraints do not limit a convex accessible domain of configuration space. Whereas the route from one equilibrium state to another, within the ASD, can be straight, it might have to follow a long and tortuous path outside the approximation. (The ASD amounts to simplify

this complex geometry, straightening up local curvatures, etc...)

Interestingly, Tkachenko and Witten [35], following a suggestion by Alexander [40], speculated that, *as a consequence of the isostaticity property*, the mechanics of frictionless sphere packings should be described, at the continuum level, by laws of the type proposed in refs. [12, 13]: the response to perturbing force fields satisfies *hyperbolic* partial differential equations. From considerations on the floppy modes that appear within a subsystem that is isolated from the rest of the sample, they derive a similar directional structure for matrix G^{-1} as for the macroscopic response in such theories: in a sample limited by a free surface in the upwards direction, force perturbations are not felt above the point where they are introduced.

Although we do not venture here to speculate on the form of macroscopic equations that rule the mechanical response with rearrangements in a general, disordered system for which the ASD might not be valid, our conclusions above do go far enough as to clearly contradict the ones of [35], since those are concerned with the same object (operator G^{-1}).

An explanation for this discrepancy could be that Tkachenko and Witten mainly based their conclusions on the observation of packings (numerically) obtained by sequential deposition algorithms under gravity.

When the stress tensor approaches the boundary of the region of supported loads (*i.e.*, when one of the conditions in 42 is almost an equality) one can observe [17], for the triangular lattice model, that the list of force-carrying contacts approaches a limit that comprises all the bonds parallel to two of the three lattice directions, and none of the bonds parallel to the third. The topology of the backbone thus approaches that of a square lattice. In this particular case [35], it is easy to check that a description in terms of *force propagation*, involving hyperbolic equations, applies. The marginally supported stress states of this model are the analog of the Coulomb condition for an isotropic medium. When the Coulomb criterion is everywhere satisfied as an equality, the material is everywhere on the verge of plastic failure, and it has long been known (and exploited for the evaluation of critical loads [53]) that the macroscopic equations are of the hyperbolic type. This situation has been termed ‘incipient failure everywhere’ (IFE) in [12, 13].

One may conjecture that deposition algorithms [54, 55] will systematically produce internal states close to IFE. Specifically, we expect sequential deposition under gravity to result in the ‘active’ Rankine state, in which the pressure on the lateral walls is barely sufficient to contain macroscopic plastic flow of a horizontal granular layer submitted to its own weight. In the case of discs with a small or moderate polydispersity in 2D, the deposition algorithms do in fact produce networks of force-carrying contacts that are very close to the limiting states of the triangular lattice model (a deformed square lattice).

Therefore, we suspect that Tkachenko and Witten’s arguments only apply to those particular cases of limit

states or IFE.

There are, apart from the arguments put forward in [35], other aspects on which the general properties we have been discussing as well as the numerical results obtained on the triangular lattice model appear at odds with the assumption of a direct relationship between stress components, and related theories. Leaving a more complete discussion to subsequent work, let us merely point out that the nature of the boundary conditions has dramatic effects if the macroscopic equations are hyperbolic. In fact, if a rigid boundary transmitting a stress is replaced by a distribution of external forces imposed independently on the grains that are close to the edge, such theories predict this change to significantly affect the whole system (which has lost its rigidity). In our experience [9, 18], some rearrangement does occur, but its effects are confined to a boundary layer of finite depth.

We also note that our results disagree with some of Moukarzel’s [33, 34], predicting perturbations due to a localized force to increase *exponentially* with distance. Although his results are very accurate and were obtained on very large systems, the *propagative* nature of forces, which can be calculated from ‘top’ to ‘bottom’ in a single sweep, is an explicit ingredient of his model, that was adapted from the one of [32]. Our results on the triangular lattice model disagree with his because this very large effect of force perturbations (or, equivalently – see 49 and 50– of bond length variations) would cause the level of distortion of the regular lattice, due to the polydispersity of discs, to increase very fast with the system size. Rather, we observed it to approach a finite thermodynamic limit. Once again, we suspect that the very peculiar properties obtained in these studies stem from the consideration of a special case in which forces happen to possess a propagative nature.

Finally, the (provisional) conclusion we propose here is, as already mentioned in section VII E, that the rigidity of the grains and the isostaticity property do not *necessarily* entail very special, critical or singular macroscopic mechanical properties. Moreover, we expect – as systems dealt with within the ASD exhibit the same kind of elasticity as networks of rigid cables – that if unusual, exotic properties exist, then they are related to the displacements (the rearrangements) rather than the network of forces (or the operator G attached to it).

X. CONCLUSION AND PERSPECTIVES.

Let us first briefly summarize the main results presented in this paper.

Specializing to frictionless grains, and assuming that granular packings, under slowly varying sollicitations, tend to stable equilibrium states, we have shown that geometry determines, to a large extent, the mechanical behaviour of such materials.

Spatial arrangements of granular packings in equilibrium under a given load are quite specific points in config-

uration space. Rigid grains that only exert normal contact forces on one another, once submitted to a supported load, will generically pack in such a way that the problem is isostatic, *i.e.*, there is no indeterminacy of forces. The value of all contact forces is determined by equilibrium equations and the geometry of the contact structure. This yields a rigourous upper bound on the contact coordination number of any packing of rigid grains. These properties hold for compressive or tensile contact forces. Contact structures, in equilibrium, are not always rigid, especially (but not exclusively) in the case when contacts can sustain tensions. Even if loose particles, that carry no force, are discarded from the count, the upper bound on the coordination number might not be reached.

If the packing is such that the approximation of small displacements might be well justified, in particular in the case of regular arrangements on lattices, stronger properties were established, provided the problem can be coped with in the framework of convex optimization theory (which requires the definition of a potential energy, thus excluding finite strength cohesion). Then

- Not only the forces once the contact structure is known, but the force-carrying structure itself is entirely determined by the system geometry.
- Grain positions are also determined, apart from possible ‘floppy mode’ motions, of bounded amplitude, that do not affect the value of the potential energy.
- Displacements from the reference configuration on the one hand, and *contact forces on the other hand* are the solutions to two optimization problems in duality.
- For rigid grains, force-carrying structures are the exact analog of cost-minimizing directed paths in scalar transport problems.

Such situations are thus very attractive from a theorist’s point of view: the reduction of the mechanical problem to one of random geometry is complete, and analogies with other models of theoretical statistical physics (directed percolation, directed polymer in a random environment) can be drawn and exploited. However some important features of granular mechanics are absent: such systems are devoid of plasticity and hysteresis.

Pursuing the stability analysis beyond the ASD in the case of discs or spheres, we have shown that the force-carrying structure must be rigid if contacts do not withstand tension, because any floppy mode would imply instability. This entails that the force-carrying backbone in systems of rigid spheres is, generically, an isostatic structure, its coordination number is equal to $2d$ in dimension d .

Analogous systems of cables (that resist tension, but no compression), on the other hand, will generally keep

some amount of floppiness, since mechanisms in the equilibrium state are all stable.

Assemblies of frictionless grains will, in general, exhibit internal friction, due to the multiplicity of stable equilibrium states corresponding to the same external load. This non-uniqueness might stem from the finite extent of rearrangements or from bounded cohesion forces.

If submitted to slowly varying loads, packings of rigid grains will evolve via a succession of jumps or crises separated by phases of rest. The isostaticity property implies, for a system of rigid frictionless spheres, that the concentration of forces is maximal during a phase of rest (forces cannot be carried by a strictly smaller set of contacts), and that the concentration of deformation is maximal at the beginning of a jump (there cannot exist a strictly smaller list of interstices in which relative normal velocities are not equal to zero).

Although the motion in a rearranging event depends on the actual granular dynamics, the forces during a phase of rest, and the direction of velocities at the beginning of motion, are geometrically determined.

Two kinds of response functions to force increments can be studied, depending on whether the perturbation provokes a change in the contact list. Some recent studies of response functions, without rearrangement of the grains, were discussed and we argued that some of their conclusions might be specific to sequential deposition models, in which forces can be propagated along a preferred direction. The fragility of frictionless granular assemblies in the thermodynamic limit implies however that macroscopically meaningful perturbations always involve some amount of rearrangement.

The results of the present article suggest both general perspectives and specific problems, to be dealt with in future work.

An important feature of granular materials is the sparsity, in configuration space, of equilibrium configurations. Those, especially for rigid grains, have very specific characteristics. Moreover, they are generally suitable for *one* particular load. In such circumstances, it might not be adequate to choose *first* one specific geometric arrangement and contact structure, built, *e.g.*, by some convenient algorithm that respects impenetrability conditions, and *then* to apply external forces and see how they could be balanced by contact forces. The list of active contacts is itself chosen according to the external load. Many recent studies were devoted to the way forces distribute among a fixed list of contacts, and to the ensuing statistics of contact force values. Although models along these lines might capture *some* of the physics, they ignore displacements. Displacements, as our results have amply shown here, are always part of the problem. The very definition of a force requires the consideration of some amount of displacement. A normal reaction force in the frictionless contact between two rigid objects is a geometrically defined quantity, a Lagrange parameter associated with an impenetrability constraint in configuration space. Large assemblies of frictionless rigid grains are fragile:

tiny load increments will be associated with rearrangements of the contact structure. If one wishes to understand the macroscopic mechanical behaviour of granular systems and its relationship to grain-scale phenomena, the question of the *magnitude* of such rearrangements, in which the system moves from an equilibrium state to another, is crucial.

Other, more specific questions, that are related to statistics and the continuum limit, naturally follow from the mechanical properties we have been presenting. When is the ASD a good approximation, apart from lattice models ? Are the same states periodically revisited in cyclic sollicitations ? What will be the density and the effect of floppy modes in systems of non-spherical frictionless particles ? Will the staircase-like stress-strain curve approach a smooth limit when the system size increases ? To what extent are rearrangements sensitive to the actual dynamical rule ? Such problems would benefit from careful numerical simulations, and we shall address some of these questions in forthcoming publications.

The treatment of granular systems with friction could be tackled with a similar approach to the one developed here: one could investigate the range of stability of a

given contact structure, as the load gradually varies, by purely static means. In the presence of friction, granular packings are also observed, in experiments and dynamic numerical simulations, to evolve by a succession of crises localized in time. We expect the geometry of the assemblage to dictate, to a large extent, the way such sudden motions are initiated.

It can be concluded that much of the promising prospects, as well as much of the difficulties ahead, in the study of mechanical properties of granular materials close to equilibrium, are in the understanding of the disordered, yet quite peculiar, geometry of large systems that adapt their contact network to sustain the load.

Acknowledgments

The author wishes to thank J.-P. Bouchaud, X. Chateau, E. Clément, G. Combe, P. Dangla, M. Jean, J. Jenkins, J.-J. Moreau, S. Ouaguenouni, F. Radjai, J. Rajchenbach and J. Socolar for stimulating contacts and conversations.

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- [56] Our considerations do apply, in fact, to flat surfaces, provided face to face contacts are counted d times in d dimensions, as they transmit one force and $d - 1$ torques.
- [57] This latter condition is not essential: the properties of Section II hold true provided the direction of the force carried by a bond is fixed.
- [58] The load, in that case, is supportable if, and only if, $42p \leq Q_1\sqrt{3} \leq 74p$
- [59] In fact, all the properties of Sections II, IV, VI hold true provided the *direction* of each intergranular force is imposed.
- [60] The interested reader might obtain the list of sphere positions from the author.
- [61] The fragility property is in fact contained in the results stated in paragraph VII.B.8, as any stress increment, however small, that is not parallel to the preexisting stress, entails some additional strain in the thermodynamic limit